Revisiting the Exact Dynamical Structure Factor of the Heisenberg Antiferromagnetic Model

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Résumé

We revisit our initial derivations of the exact 2-spinon S_2 and 4-spinon S_4 dynamical structure factors (DSF). First we show that the latter derivations had normalization factors that are twice and quadriple the correct ones respectively. This means that S_2 contributes not 72% as was previously thought but 36% to the total DSF. We also calculated the contribution of S_4 to be between 18% and 20% and not 27% as was calculated by Caux and Hagemans. In fact we show that the latter reference had also the normalization factor twice the correct value and had it done the numeric integrations correctly it would have obtained a contribution between 36% and 40% for S_4. Furthermore, we prove that its claim that our initial derivation of S_4 was also incorrect in its dependency on the spectral parameters is incorrect because fixing the momentun transfer k up to 2π as the latter reference did to justify its claim only amounts to mutltiplying the overall factor by 2 because as we will prove in this paper S_4 is periodic in k with period 2π. Also in this paper we derive S_n for general n by following a different approach compared to our initial derivation of S_4. Although for S_4 both the new derivation and the initial one lead to equivalent formulas that are expressed differently, the new form presented in this paper is much more elegant and compact and also reveals new hidden and nontrivial symmetries which substantially simplify the numeric evaluation of S_4 and its sum rules. Moreover based on the results of this paper we propose a simple approximation to the total DSF of the Heisenberg model. Finally we comment on how our work might resolve the discrepancy between the exact theoretic results and experiemntal data as reported by Zaliznyak et al.

1 Introduction

It is well known that the family of 1D quantum spin chain models play a crucial role both from a physical point of view and a mathematical point of view as they lend themselves to exact solutions based on mathematical algebraic theories and they lend themselves to precise experiments in the lab [1-15]. This is due to the fact that these models exhibit symmetries that can be described rigourously by well known algebras and their spectrum of enseigenspaces can be built from well structured representations of these algerbras. Moreover in the thermodynamic limit, the symmetries of these models become infinite dimensional meaning that the latter models must satisfy an infinite number of constraints. Because of this only a finite number of representations survive, thus making these models exactly and completely solvable. By completely solvable we mean not only can we describe exactly their eigenspaces but also exactly calculate the physical quantities such as the S matrix, the form factors of their local operators, and the static

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and dynamic correlation functions. Although in the latter case the physical quantities are often expressed as sums of infinite series they nonetheless often converge and only a finite number of terms contribute to any given precision. This is to be contrasted with the finite chains case where the symmetries are described by finite algebras having an infinite number of representations thus rendering these models not completely and exactly solvable. The model by excellence that embodies this phenomenon is the anisotropic Heisenberg chain in the thermodynamic limit which was shown in [12],[13] to be symmetric under the infinite dimensional quantum affine algebra $U_q(\widehat{sl}(2))$. Since this algebra has only two representations therefore this model is exactly solvable. Indeed the static correlation functions and the form factors were exactly calculated in [13]. Based on them the dynamical structure factors (DSF) due to 2 spinons and 4 spinons were exactly calculated in [16] and [17] respectively. Further studies in [18] and [19] using the sum rules showed that the 2-spinon DSF contributes 72% and the 4-spinon DSF contributes 27% to the total DSF, respectively. This would then mean that the contributions of both S_2 and S_4 would account for 99% of the total DSF. However experiemental data obtained in [20] and [21] reveal that the observed contribution accounts roughly only for the third of the total theoretic DSF. Motivated by these experimental data and the inconsistency they raised with respect to the currently available exact theoretic results we decided to reexamine our initial derivations of the 2-spinon DSF in [16] and 4-spinon DSF in [17] and to relate them as a consistency check to the exact static correlation functions obtained in [13] and [22]. The main conclusion we reach and that we will explain in details in this paper is that the normalisation overall factor of S_2 was ove-revaluated by a factor 2 in [16] and the normalisation overall factor of S_4 was also overevaluated by a factor of 4 in [17] and by a factor of 2 in [19]. This means S_2 contributes 36% instead of 72% and the 4-spinon DSF contributes $18-20\%$ instead of 27% to the total DSF, respectively. In fact we believe that if the numeric calculation was done correctly in [19] they would have obtained a contribution of $36\% - 40\%$ and not 27%. This would have been a major inconsistency since at that time S_2 was believed to contribute already 72% which means that S_2 and S_4 together would contribute more than 100% which obviously is impossible. Therefore one of the results of the present paper is then the contributions of S_2 and S_4 add up to only $54-56\%$. We believe that the observed DSF as reported in [20], [21] which accounts for the third of the total DSF would be just the contribution of S_2 which we found to be 36% which is roughly the third of 100%.

Unlike our original derivations of S_2 and S_4 where we have calculated them first in the anisotrpic case and then taken the istropoic limit at the last stage, this time around we decided to derive S_n for the general case of n spinons by starting out from the form factors directly in the isotropic limit. In the latter limit the form factors are expressed as integrals in the case of $n \geq 4$ but they have an incorrect overall factor in [13] that we correct in this paper. We then analytically integrate the latter integrals explicitly. We get the same expression for S_2 as before but for S_4 we get a new formula that is equivalent to the old one but expressed in a different form. In particular our new derivation highlights the existence of hidden structures represented by the appearance of a new vector of function elements and a new matrix of function elements in terms of which S_4 is simply expressed. Both the latter function elements satisfy highly nontrivial symmetry relations with respect to the permutations of both their spectral parameters and their indices which identify the 4 spinons. As a byproduct of these symmetries which translate into a simple expression of S_4, the actual numerical computation for the purpose of sum rules and for the purpose of graphical plotting of S_4 are greatly simplified as we will see in the main text. As a new result presented in this paper we show that in the general case of S_n the overall normalisation factor can be expressed simply in terms of the Glaisher-Kinkelin constant and only in the case of S_2 does this constant cancel out leading to a simple overall factor of $1/4$. This provides an analytic proof why the S_2 normalisation factor is exactly equal to $1/4$, a result which as far

as we know was only derived numerically in [18].

We make a comment on the expression for S_4 presented in [19] by noting that it is the same as the one originally computed by us in [17] up to an overall factor. To be more precise in [17] we had an incorrect extra multiplicative factor of 2 from adding contributions to the DSF from both sectors $i = 0, 1$ corresponding to the two possible representations of $U_q(\widehat{sl(2)})$, and an incorrect extra mutlipliticative factor of 4 from expressing the sums of exponentials of the energy terms and the sums of exponentials of the momenta terms in terms of the delta functions, and a missing multiplicative factor of 2 from the possibility of fixing the spinon momenta only up to 2π. The reason why the last error amounts only to a missing 2 mutliplicative factor is that in general S_n is periodic with respect to the momentum transfer and spinon momenta with period 2π. Therefore adding the contribution of the DSF when one of the spinon momenta is shifted by 2π (which in turn amounts to shifting the momentun transfer by 2π) simply amounts to a mutltiplicative overall factor of 2. In [19] they justified the latter contribution by saying that the delta function fixes the momentum transfer only up to 2π but in fact it is not the momentun transfer that is fixed up to 2π and which should be exactly fixed but it is rather the momenta of the spinons which are fixed up to 2π. Also in the latter reference it is not clear why they have not used the same argument with respect to the delta function of the energies to justify a fixing of the energy transfer only up to 2π in a similar manner as they did for the momenta. In fact part of our analysis is to prove that there is an asymmetry between the momenta of the spinons which are fixed only up to 2π and the energies of the spinons which are exactly fixed. Also in this reference the authors proposed an overall factor in an ad hoc manner without any justification of its derivation from first principles as we do in this paper but their overall factor also has the incorrect extra multiplicative factor of 2 from adding contributions to the DSF from both sectors of the eigenspace. Finally we also believe that their numerics are less precise when its comes to the computation of the sum rules in that they found S_4 to account for 27% when they should have found somewhere between 36% and 40%. So to sum up in the case of S_4 our initial paper [17] had an incorrect extra mutliplicative factor of 4 in its normalization factor, whereas the paper in [19] has an incorrect multiplicative factor of 2 and less precise numeric evaluations of the sum rules. We also compare our initial expression for S_4 with the one used in [23] and conclude that their expression used a incorrect overall normalisation factor to start with and also their Monte Carlo integration was incorrect.

Since in this paper we show that S_2 and S_4 saturate the total DSF only up to $54\% - 56\%$ we need therefore to study the higher sectors as well. From the shapes of S_2 and S_4 as functions of energy transfer for fixed momentum transfer one can notice that they are very similar in that S_4 almost looks like a scaled down version of S_2 in the common first Brouillin zone $[0, 2\pi]$. Beyond $[0, 2\pi]$ S_2 is null and S_4 is extremely small. One is tempted then to conclude that this pattern would still hold true for the general S_n. Since S_2 is the only one which is very simple and expressed as a single term and captures the general shape of the general S_n up to a scale factor we propose then an approximation to the total DSF as a scaled up version of S_2 such that it saturates the sum rules. This approximation is somewhere in the middle between the Muller ansatz and the exact one. It is better than the Muller anstaz because it has a much better shape that closely fits the experimental data and it is almost as simple as the Muller anstaz, and also it is much simpler that the exact total DSF which is very complex. The only drawback is that it misses all the spectral weight beyond the first Brouillin zone of $[0, 2\pi]$ although the latter is negligeable for general n.

Finally we note that in this paper for the purpose of plotting S_4 and calculating its sum rules

we have used the Genz-Malik adaptive algorithm [24] for evaluating high dimensional integrals. As discussed in [25] the initial Genz-Malik adaptive integration method and its Berntsen-Espelid-Genz [26] enhanced version are highly superior to Monte Carlo or Quasi Monte Carlo methods because the latter can be ineffecient if most of the randomly generated points lie outside the region where the integrand contributes the most to the integral. Even the better uniform properties of quasi-Monte Carlo sequences over Monte Carlo simulation can also be useless. In addition, both Monte Carlo and quasi-Monte Carlo methods are not able to take advantage of the regular behavior of the integrand. However, the Genz-Malik adaptive integration algorithm can be highly superior to Monte Carlo and quasi-Monte Carlo methods because it successively divides the integration region into subregions and detects the subregions where the integrand is most irregular (such as functions with peaks, singular points, discontinuities, oscillatory) and therefore places more points in those subregions. The Berntsen-Espelid-Genz enhanced version of the latter algorithm has a more sophisticated algorithm for the error estimation. The only disadvatange of the adaptive algorithms compared to Monte Carlo and Quasi Monte Carlo is that they do no scale well to very high dimensions because the number of evaluation points in each subregion increases exponentially, thus facing the dreaded curse of dimensionality again. In fact they are useful for small to moderate number of dimensions from 2 to 11, beyond which Monte Carlo and Quansi Monte Carlo are still the better option. Since in this paper we are faced with 2d integrations for S_4 and the sum rules of S_2, and 4d integration of the sum rules of S_4 we use the adaptive Berntsen-Espelid-Genz algorithm.

This paper is organized as follows in section 2. we compute analytically S_n DSF for the general case of n spinons and then we specialize it to 2-spinon et 4-spinon cases. Here we also prove that the physical DSF is obtained only from one sector of the eigenspace and not both sectors as was incorrectly done in our initial derivation. In section 3. we study the sum rules of S_2, S_4 and S_n in general. In particular we show that S_2 contributes 36% and S_4 contributes between 18% and 20% depending on which sum rule is used. In section 4. we present our approximate total DSF of the Heisenberg model. Finally in section 5. we present our conclusions.

2 n-spinon DSF

The Hamiltonian of the anisotropic (XXZ) Heisenberg model is defined by

$$H_{XXZ} = -\frac{1}{2}\sum_{n=-\infty}^{\infty}(\sigma_n^x\sigma_{n+1}^x + \sigma_n^y\sigma_{n+1}^y + \Delta\sigma_n^z\sigma_{n+1}^z), \tag{1}$$

where $\Delta = (q + q^{-1})/2$ is the anisotropy parameter. Here $\sigma_n^{x,y,z}$ are the usual Pauli matrices acting at the n^{th} position of the formal infinite tensor product

$$W = \cdots V \otimes V \otimes V \cdots, \tag{2}$$

where V is the two-dimensional representation of $U_q(sl(2))$ quantum group. We consider the model in the anti-ferromagnetic regime $\Delta < -1$, i.e., $-1 < q < 0$. Refs. [12, 13] diagonilized H_{XXZ} in terms of the set of eigenstates (spinons) denoted by $\mathcal{F} = \{|\xi_1, \cdots \xi_n >_{\epsilon_1,\cdots\epsilon_n;i}, n \geq 0, \quad i = 0, 1\}$. Here i fixes the boundary conditions such that the allowable spin configurations are those for which the eigenvalues of σ_n^z are $(-1)^{i+n}$ in the limit $n \to \pm\infty$. ξ_j are the spectral parameters living on the unit circle, and $\epsilon_j = \pm 1$ are the spins of the spinons. The actions of

H_{XXZ} and the translation operator T, which shifts the spin chain by one site, on $\mathcal{F}$ are given by

$$\begin{array}{rcl} T|\xi_1, \cdots, \xi_n >_i &=& \prod_{i=1}^{n} \tau(\xi_i)^{-1} |\xi_1, \cdots, \xi_n >_{1-i}, \quad T|0>_i = |0>_{1-i}, \\ H_{XXZ}|\xi_1, \cdots, \xi_n >_i &=& \sum_{i=1}^{n} e(\xi_i) |\xi_1, \cdots, \xi_n >_i, \end{array} \tag{3}$$

where

$$\begin{array}{rcl} \tau(\xi) &=& \xi^{-1} \frac{\theta_{q^4}(q\xi^2)}{\theta_{q^4}(q\xi^{-2})} = e^{-ip(\alpha)}, \quad p(\alpha) = am(\frac{2K}{\pi}\alpha) - \pi/2, \\ e(\alpha) &=& \frac{1-q^2}{2q} \xi \frac{d}{d\xi} \log \tau(\xi) = \frac{2K}{\pi} \sinh(\frac{\pi K'}{K}) dn(\frac{2K}{\pi}\alpha). \end{array} \tag{4}$$

Here, $e(\alpha)$ and $p(\alpha)$ are the energy and the momentum of the spinon respectively, $am(\alpha)$ and $dn(\alpha)$ are the usual elliptic amplitude and delta functions respectively, with the complete elliptic integrals of the first kind K and K', and

$$\begin{array}{rcl} q &=& -\exp(-\pi K'/K), \\ \xi &=& ie^{i\alpha}, \\ \theta_x(y) &=& (x;x)_\infty (y;x)_\infty (xy^{-1};x)_\infty, \\ (y;x)_\infty &=& \prod_{n=0}^{\infty} (1 - yx^n). \end{array} \tag{5}$$

Thus the anisotropic parameter q in the anisptropic Heisenberg model XXZ plays also the dual role of being the nome of the latter elliptic functions and the deformation parameter of the quantum group $U_q(\widehat{sl}(2))$ under which XXZ is symmetric. The local operators $\sigma^{x,y,z}(t,n)$ at time t and position n are related to $\sigma^{x,y,z}(0,0)$ at time 0 and position 0 through :

$$\sigma^{x,y,z}(t,n) = \exp(itH_{XXZ}) T^{-n} \sigma^{x,y,z}(0,0) T^n \exp(-itH_{XXZ}). \tag{6}$$

The completeness relation over $\mathcal{F}$ reads [13] :

$$I = \sum_{i=0}^{1} \sum_{n=0}^{\infty} \sum_{\epsilon_1, \cdots, \epsilon_n = \pm 1} \frac{1}{n!} \oint \frac{d\xi_1}{2\pi i \xi_1} \cdots \frac{d\xi_n}{2\pi i \xi_n} |\xi_n, \cdots, \xi_1 >_{\epsilon_n, \cdots, \epsilon_1; i} \ {}_{i; \epsilon_1, \cdots, \epsilon_n}< \xi_1, \cdots, \xi_n|. \tag{7}$$

where I is the identity operator acting on $\mathcal{F}$. In the case of the anisotrpoic XXZ model the dynamic structure function (DSF) corresponding to the operators $\sigma^{\pm} = (\sigma^x \pm i\sigma^y)/2$) and to the sector i of $\mathcal{F}$ is defined by :

$$S^{i,+-}(w,k) = \int_{-\infty}^{\infty} dt \sum_{m \in Z} e^{i(wt+km)} {}_i< 0|\sigma^+(t,m)\sigma^-(0,0)|0 >_i, \tag{8}$$

where in the above Fourier transform w and k are the energy and momentum transfer respectively, and Z is the set of integers. As we will see later it turns out that the DSF is in fact independent of i and therefore is the same for both sectors. One can always insert the identity operator between the operators $\sigma^+(t,n)$ and $\sigma^-(0,0)$ in (8) without affecting the value of $S^{i,+-}(w,k)$, that is :

$$S^{i,+-}(w,k) = \int_{-\infty}^{\infty} dt \sum_{m \in Z} e^{i(wt+km)} {}_i< 0|\sigma^+(t,m) I \sigma^-(0,0)|0 >_i . \tag{9}$$

Substituting in the latter relation the identity operator I by the right hand side of the completeness relation (7) we find :

$$S^{i,+-}(w,k) = \sum_{n=0}^{\infty} S_n^{i,+-}(w,k), \tag{10}$$

with the n-spinon DSF $S_n^{i,+-}(w,k)$ being defined by :

$$\begin{array}{rcl} S_n^{i,+-}(w,k) & = & \frac{1}{n!}\sum_{\epsilon_1,\cdots,\epsilon_n=\pm 1}\oint\frac{d\xi_1}{2\pi i\xi_1}\cdots\frac{d\xi_n}{2\pi i\xi_n} \\ & & \times\int_{-\infty}^{\infty}dt\sum_{m\in Z}e^{i(wt+km)} \\ & & \times_i<0|\sigma^+(t,m)|\xi_n,\cdots,\xi_1>_{\epsilon_n,\cdots,\epsilon_1;i}\ {}_{i;\epsilon_1,\cdots,\epsilon_n}<\xi_1,\cdots,\xi_n|\sigma^-(0,0)|0>_i, \end{array} \tag{11}$$

where we have used the orthogonality relations [13] :

$$\begin{array}{rcl} {}_i<0|\sigma^+(t,m)|\xi_n,\cdots,\xi_1>_{\epsilon_n,\cdots,\epsilon_1;j} & = & \delta_{ij}\times{}_i<0|\sigma^+(t,m)|\xi_n,\cdots,\xi_1>_{\epsilon_n,\cdots,\epsilon_1;i} \\ {}_{j;\epsilon_1,\cdots,\epsilon_n}<\xi_1,\cdots,\xi_n|\sigma^-(0,0)|0>_i & = & \delta_{ij}\times{}_{i;\epsilon_1,\cdots,\epsilon_n}<\xi_1,\cdots,\xi_n|\sigma^-(0,0)|0>_i, \end{array} \tag{12}$$

with the usual Kronecker symbol defined by $\delta_{ii}=1$ and $\delta_{ij}=0$ if $i\neq j$. $S_n^{i,+-}$ can be expressed through (3) and (6) as :

$$\begin{array}{rcl} S_n^{i,+-}(w,k) & = & \frac{1}{n!}\sum_{\epsilon_1,\cdots,\epsilon_n=\pm 1}\oint\frac{d\xi_1}{2\pi i\xi_1}\cdots\frac{d\xi_n}{2\pi i\xi_n} \\ & & \times\int_{-\infty}^{\infty}dt\exp\left(it(w-\sum_{\ell=1}^n e(\xi_\ell))\right) \\ & & \times\sum_{m\in Z}\left(\exp\left(im(k+\sum_{\ell=1}^n p(\xi_\ell)\right)\right) \\ & & \times_{i+m}<0|\sigma^+(0,0)|\xi_n,\cdots,\xi_1>_{\epsilon_n,\cdots,\epsilon_1;i+m}\ {}_{i;\epsilon_1,\cdots,\epsilon_n}<\xi_1,\cdots,\xi_n|\sigma^-(0,0)|0>_i). \end{array} \tag{13}$$

Given the fact that there are only 2 sectors $i=0,1$ and therefore the sectors $i+m$ are defined only modulo 2, we can split the sum over Z in terms of even elements and odd elements and rewrite the latter formula as :

$$\begin{array}{rcl} S_n^{i,+-}(w,k) & = & \frac{1}{n!}\sum_{\epsilon_1,\cdots,\epsilon_n=\pm 1}\oint\frac{d\xi_1}{2\pi i\xi_1}\cdots\frac{d\xi_n}{2\pi i\xi_n} \\ & & \times\int_{-\infty}^{\infty}dt\exp\left(it(w-\sum_{\ell=1}^n e(\xi_\ell))\right) \\ & & \times\sum_{m\in Z}\left(\exp\left(2im(k+\sum_{\ell=1}^n p(\xi_\ell))\right)\right) \\ & & \times\left({}_i<0|\sigma^+(0,0)|\xi_n,\cdots,\xi_1>_{\epsilon_n,\cdots,\epsilon_1;i}\ {}_{i;\epsilon_1,\cdots,\epsilon_n}<\xi_1,\cdots,\xi_n|\sigma^-(0,0)|0>_i\right. \\ & & +\exp\left(i(k+\sum_{\ell=1}^n p(\xi_\ell)\right) \\ & & \times\ {}_{1-i}<0|\sigma^+(0,0)|\xi_n,\cdots,\xi_1>_{\epsilon_n,\cdots,\epsilon_1;1-i}\ {}_{i;\epsilon_1,\cdots,\epsilon_n}<\xi_1,\cdots,\xi_n|\sigma^-(0,0)|0>_i). \end{array} \tag{14}$$

To simplify the latter expression even further we use the fact that the form factors of the operators σ^+ and σ^- satisfy the following relations [13] :

$$\begin{array}{rcl} {}_{i;\epsilon_1,\ldots,\epsilon_n}<\xi_1,\ldots.,\xi_n|\sigma^-(0,0)|0>_i & = & \left({}_i<0|\sigma^+(0,0)|\xi_n,\ldots.,\xi_1>_{\epsilon_n,\ldots.,\epsilon_1;i}\right)^* \\ {}_i<0|\sigma^+(0,0)|\xi_n,\ldots.,\xi_1>_{\epsilon_n,\ldots.,\epsilon_1;i} & = & 0\text{ if }\sum_{l=1}^n\epsilon_l\neq -2. \end{array} \tag{15}$$

The last relation means that only $S_n^{i,+-}$ with n even are non-vanishing. Using the latter relations and for a reason that will make sense later when we consider the form factors in the isotropic limit we shift k by π to get :

$$\begin{array}{rcl} S_n^{i,+-}(w,k-\pi) & = & \frac{1}{n!}\sum'_{\epsilon_1,\cdots,\epsilon_n=\pm 1}\oint\frac{d\xi_1}{2\pi i\xi_1}\cdots\frac{d\xi_n}{2\pi i\xi_n} \\ & & \times\int_{-\infty}^{\infty}dt\exp\left(it(w-\sum_{\ell=1}^n e(\xi_\ell))\right) \\ & & \times\sum_{m\in Z}\left(\exp\left(2im(k+\sum_{\ell=1}^n p(\xi_\ell))\right)\right) \\ & & \times\left(|{}_i<0|\sigma^+(0,0)|\xi_n,\cdots,\xi_1>_{\epsilon_n,\cdots,\epsilon_1;i}|^2\right. \\ & & -\exp\left(i(k+\sum_{\ell=1}^n p(\xi_\ell))\right) \\ & & \left.\times\ {}_{1-i}<0|\sigma^+(0,0)|\xi_n,\cdots,\xi_1>_{\epsilon_n,\cdots,\epsilon_1;1-i}\ \left({}_i<0|\sigma^+(0,0)|\xi_n,\cdots,\xi_1>_{\epsilon_n,\cdots,\epsilon_1;i}\right)^*\right). \end{array} \tag{16}$$

Here by the symbol $\sum'_{\epsilon_1,\cdots,\epsilon_n=\pm 1}$ we mean the sum is constrained by the selection rule expressed by the second relation in (15). Now we will take the isotropic limit of the XXZ Heisenberg model

where the latter formula will simplify even further. The isotropic limit $q \to -1$ is performed by first making the following redefinitions :

$$\begin{array}{rcl} \xi & = & i e^{\frac{\epsilon \beta}{i\pi}}, \\ q & = & -e^{-\epsilon}, \quad \epsilon \to 0^+, \end{array} \tag{17}$$

where β is the spectral parameter corresponding to the isotropic Heisenberg model. Then, we find in this limit [13] :

$$\begin{array}{rcl} & & {}_i\!< 0|\sigma^+(0,0)|\xi_n, ..., \xi_1 >_{\epsilon_n,...,\epsilon_1;i} \\ & \to & {}_i\!< 0|\sigma^+(0,0)|\beta_n, ..., \beta_1 >_{\epsilon_n,...,\epsilon_1;i} \\ & \to & -{}_{1-i}\!< 0|\sigma^+(0,0)|\beta_n, ..., \beta_1 >_{\epsilon_n,...,\epsilon_1;1-i} \\ & \sim & \epsilon^{-n/2} C_{1,i,n} \\ & & \times \prod_{m>\ell=1}^{n} \frac{A_-(\beta_m-\beta_\ell)}{A_-(\pi i/2)\Gamma(1/4)} \prod_{\ell=1}^{n} \frac{\pi i}{\sinh(\pi i/4-\beta_\ell/2)} \\ & & \times \prod_{b\in B} \Big(\int_{\bar{C}_b} \frac{d\alpha_b}{2\pi i} \\ & & \times \prod_{\ell=1}^{b-1} (\alpha_b - \beta_\ell + \frac{\pi i}{2}) \prod_{\ell=b+1}^{n} (\beta_\ell - \alpha_b + \frac{\pi i}{2}) \\ & & \times \prod_{\ell=1}^{n} \Gamma(-\frac{1}{4} + \frac{\alpha_b-\beta_\ell}{2\pi i}) \Gamma(-\frac{1}{4} - \frac{\alpha_b-\beta_\ell}{2\pi i}) \\ & & \times \sinh(\alpha_b) \\ & & \times \prod_{b'\in B, b'>b} (\alpha_b - \alpha_{b'} + \pi i) \sinh(\alpha_b - \alpha_{b'}) \Big), \\ C_{1,i,n} & = & i^{n^2/4+n-2i} 2^{-3n^2/4+n/2} \pi^{-7n^2/8+9n/4-1} \Gamma(3/4)^{-n/2} A_+(\pi i/2)^{-n/2}, \\ p(\xi_\ell) & \to & p(\beta_\ell), \quad \cot(p(\beta_\ell)) = \sinh(\beta_\ell), \quad -\pi \le p(\beta_\ell) \le 0, \\ e(\xi_\ell) & \to & e(\beta_\ell) = \frac{\pi}{\cosh(\beta_\ell)} = -\pi \sin(p(\beta_\ell)), \quad 0 \le e(\beta_\ell) \le \pi, \quad 1 \le \ell \le n, \\ \oint \frac{d\xi_1}{2\pi i \xi_1} ... \oint \frac{d\xi_n}{2\pi i \xi_n} & \to & \epsilon^n 2^{-n} \pi^{-2n} \int_{-\infty}^{+\infty} d\beta_1 ... \int_{-\infty}^{+\infty} d\beta_n, \end{array} \tag{18}$$

where the set B associated with a configuration $(\epsilon_n, ..., \epsilon_1)$ is defined by

$$\begin{array}{rcl} B & = & \{b; \quad \epsilon_b = +1; \quad \sum_{\ell=1}^{n} \epsilon_\ell = -2\}, \\ \dim\,(B) & = & n/2 - 1 \equiv N. \end{array} \tag{19}$$

The contours $\bar{C}_b$ are drawn in Figure 1. In the expression of $C_{1,i,n}$ and more precisely in $(i)^{-2i}$, the i that is in the exponent refers to the sector index (i.e., $i = 0, 1$), whereas the i that is not in the exponent refers to the unit complex imaginary number (i.e. $i^2 = -1$). Also in all terms πi, i refers to the unit complex imaginary number. Note that there was an error in the formula of $C_{1,i,n}$ given in [13], and which has been corrected in the above expression by having $C_{1,i,n}$ proportional to the factor $\Gamma(3/4)^{-n/2}$ instead of $\Gamma(3/4)^{n/2}$ as was incorrectly done in [13]. Finally $\Gamma(z)$ is the usual gamma function and for a complex variable $z = x + iy$, with x and y being real, the complex functions $A_\pm(z)$ and their square modulus $|A_\pm(z)|^2$ are defined in terms of the following integrals :

$$\begin{array}{rcl} A_\pm(z) & = & \exp\Big(-\int_0^\infty dt \frac{\sinh^2(t(1-\frac{z}{\pi i}))}{t \sinh(2t)\cosh(t)} \exp(\mp t) \Big), \\ |A_\pm(z)|^2 & = & \exp\Big(-\int_0^\infty dt \frac{(\cosh(2t(1-\frac{y}{\pi}))\cos(\frac{2tx}{\pi})-1)}{t \sinh(2t)\cosh(t)} \exp(\mp t) \Big). \end{array} \tag{20}$$

From the latter relation one can show that the following constant terms which contribute to the overall normalization factor of $S_n^{i,+-}$ can be expressed as :

$$\begin{array}{rcl} |A_\pm(i\pi/2)|^2 & = & \exp\Big(-\int_0^\infty dx \frac{\cosh(x)-1}{x \sinh(2x)\cosh(x)} \exp(\mp x) \Big) = \pi \Gamma(1/2 \pm 1/4)^{-2} \left(\sqrt[6]{2}\sqrt{e} A^{-6} \right)^{\pm 1}, \\ A & = & \exp\big(\frac{1}{12} - \zeta'(-1) \big) = 1.2824271291 \cdots, \end{array} \tag{21}$$

where A is the Glaisher-Kinkelin constant and $\zeta(x)$ is the usual Riemann zeta function. Since as we will see later the final formula of $S_n^{i,+-}$ will be expressed just in terms of $|A_-(\beta)|^2$ with the spectral parameter β being real let us then define for the sake of simplifying the notation the real valued function $A(\beta)$ that we refer to henceforth as the "Jimbo Miwa function" (since they were the first aiuthors to introduce it and this function seems to be an extremely important one in terms of which the Heisenberg model is exactly solved) as :

$$A(\beta) \equiv |A_-(\beta)|^2 = \exp\left(-\int_0^\infty dt \frac{(\cosh(2t)\cos(\frac{2t\beta}{\pi}) - 1)}{t\sinh(2t)\cosh(t)}\exp(t)\right). \tag{22}$$

From (18) the isotropic limit of $S_n^{i,+-}$ as given by (16) is equal to :

$$\begin{array}{rcl} S_n^{i,+-}(w, k-\pi) & \rightarrow & \epsilon^n C_{2,n} \sum'_{\epsilon_1,\cdots,\epsilon_n} \int_{-\infty}^{+\infty} d\beta_1 \cdots \int_{-\infty}^{+\infty} d\beta_n \\ & & \times \left(\sum_{m\in Z}\left(\exp\left(2im(k + \sum_{\ell=1}^n p(\beta_\ell)\right)\right)\right) \\ & & \times \left(\int_{-\infty}^{\infty} dt \exp\left(it(w - \sum_{\ell=1}^n e(\beta_\ell))\right)\right) \\ & & \times|_i < 0|\sigma^+(0,0)|\beta_n, \cdots, \beta_1 >_{\epsilon_n,\ldots,\epsilon_1;i}|^2 \\ & & \times\left(1 + \exp\left(i\left(k + \sum_{\ell=1}^n p(\beta_\ell)\right)\right)\right), \end{array} \tag{23}$$

with

$$C_{2,n} = 2^{-n}\pi^{-2n}(n!)^{-1}. \tag{24}$$

Now a source of an error that plugged all existing papers dealing with the exact DSF in that they all got the normalization overall factor incorrect is due to the tricky step of expressing each of following sum : $\sum_{m\in Z}\exp(2im(k + \sum_{\ell=1}^n p(\xi_\ell))$ and integral : $\int_{-\infty}^{\infty} dt \exp it(w - \sum_{\ell=1}^n e(\xi_\ell))$ in terms of the usual Dirac delta function $\delta(x)$. The difficuly lies in the fact that the Dirac delta function is not really a function but to be more precise a distribution that can be thought of just by what it does to other usual functions as opposed to any intrinsic and explicit functional form. Except for the 2-spinon DSF, all the current papers in the litterature used incorrect normalization factors when they expressed the latter sum and integral in terms of the delta function. For this reason we decided to take a disgrression and study as rigourously as possible this issue. For this we recall the following exact result relating sum of exponentials to the delta function as described in [27] :

$$\begin{array}{rcl} lim_{M->\infty}\sum_{m=-M}^{M}\exp imx & = & 2\pi\sum_{\ell'=0}^{\ell-1}\delta(x - 2\pi\ell'), \quad 0 \le x \le 2\pi\ell, \\ lim_{M->\infty}\sum_{m=-M}^{M}\exp imx & = & 2\pi\sum_{\ell'=-\ell+1}^{0}\delta(x - 2\pi\ell'), \quad -2\pi\ell \le x \le 0. \end{array} \tag{25}$$

Let us note that the momenta $-\pi \le p(\beta_\ell) \le 0$, $\ell = 1, \cdots, n$ of n spinons are defined only modulo 2π inside the domain of definition of the total momentum of n spinons $-k = \sum_{\ell=1}^n p(\beta_\ell) \in [-n\pi, 0]$. However the energies $0 \le e(\beta_\ell) \le \pi$, $\ell = 1, \cdots, n$ are not defined modulo 2π inside the domain of definition of the total energy of n spinons $w = \sum_{\ell=1}^n e(\beta_\ell) \in [0, n\pi]$. Since we will be integrating over the two momenta $p(\beta_1)$ and $p(\beta_2)$ and thus the two corresponding energies $e(\beta_1)$ and $e(\beta_2)$ we have then from (25) :

$$\begin{array}{rcl} \int_{-\infty}^{\infty} dt \exp it(w - \sum_{\ell=1}^n e(\beta_\ell)) & = & 2\pi\delta(w - \sum_{\ell=1}^n e(\beta_\ell)), \quad 0 \le e(\beta_1) + e(\beta_2) \le 2\pi, \\ \sum_{m\in Z}\exp 2im(k + \sum_{\ell=1}^n p(\beta_\ell)) & = & 2\pi\sum_{\ell'=-n/2+1}^{0}\delta(2(k + \sum_{\ell=1}^n p(\beta_\ell) - 2\pi\ell')) \\ & = & \pi\sum_{\ell'=-n/2+1}^{0}\delta(k + \sum_{\ell=1}^n p(\beta_\ell) - 2\pi\ell'), \\ & & \quad -n\pi \le p(\beta_1) + p(\beta_2) \le 0. \end{array} \tag{26}$$

Now in the last relation one can always shift the momenta of the spinons to cancel the term $2\pi\ell'$ in $\delta(k + \sum_{\ell=1}^n p(\beta_\ell) - 2\pi\ell')$ thus effectively leading to the following final form of formulae

relating the sum $\sum_{m\in Z}\exp(2im(k+\sum_{\ell=1}^{n}p(\xi_\ell))$ and integral $\int_{-\infty}^{\infty}dt\exp it(w-\sum_{\ell=1}^{n}e(\xi_\ell))$ to the delta function $\delta(x)$:

$$\begin{array}{rcl}\int_{-\infty}^{\infty}dt\exp it(w-\sum_{\ell=1}^{n}e(\beta_\ell)) &=& 2\pi\delta(w-\sum_{\ell=1}^{n}e(\beta_\ell)),\quad 0\leq e(\beta_1)+e(\beta_2)\leq 2\pi \\ \sum_{m\in Z}\exp 2im(k+\sum_{\ell=1}^{n}p(\beta_\ell)) &=& \frac{n\pi}{2}\delta(k+\sum_{\ell=1}^{n}p(\beta_\ell)),\quad -n\pi\leq p(\beta_1)+p(\beta_2)\leq 0.\end{array} \tag{27}$$

It was possible to make the last shift in the spinon momenta because

$$\begin{array}{rcl}\beta_\ell(p_\ell+2\pi) &=& \beta_\ell(p_\ell), \\ e(p_\ell+2\pi) &=& e(p_\ell),\quad \ell=1,\cdots,n\end{array} \tag{28}$$

and therefore the integrand of the expression (23) is periodic in the spinon momenta and k with period 2π since it depends just on the β_ℓ and delta functions. Therefore $S_n^{i,+-}(w,k-\pi)$ is also periodic in the spinon momenta and k with period 2π :

$$S_n^{i,+-}(w,k-\pi+2\pi)=S_n^{i,+-}(w,k-\pi). \tag{29}$$

It is worth mentioning that in the case of 4 spinons the authors of [19] assumed $S_4^{i,+-}(w,k-\pi)$ and $S_4^{i,+-}(w,k-\pi+2\pi)$ to be different and therefore they evaluated them separately and because of this they concluded that our initial formula derived in [17] was incorrect in its dependency on the spectral parameters β_ℓ. If fact we have just proved that $S_4^{i,+-}(w,k-\pi)=S_4^{i,+-}(w,k-\pi+2\pi)$ and therefore our initial formula was incorrect just by factor of 2 in its overall factor and its dependency on the spectral parameters β_ℓ was indeed correct contrary to the claim of [19]. Also note that in [19] the authors justified the inclusion of the contribution $S_4^{i,+-}(w,k-\pi+2\pi)$ by saying that the delta function fixes the momentum transfer k only up to 2π but in fact it is not the momentun transfer that is fixed up to 2π and which should be exactly fixed but it is rather the momenta of the spinons which are fixed up to 2π. Also in the latter reference it is not clear why the authors have not used the same argument with respect to the delta function of the energies to justify a fixing of the energy transfer only up to 2π in a similar manner as they did for the momenta. We have just proved that there is an asymmetry between the momenta of the spinons which are fixed only up to 2π and the energies of the spinons which are exactly fixed. So if we make usage of (27) back in (23) we obtain :

$$\begin{array}{rcl}S_n^{i,+-}(w,k-\pi) &\to& \epsilon^n\frac{C_{3,n}}{2}\sum'_{\epsilon_1,\cdots,\epsilon_n}d\beta_1\cdots\int_{-\infty}^{+\infty}d\beta_n \\ && \times\delta\left(w-\sum_{\ell=1}^{n}e(\beta_\ell)\right)\delta\left(k+\sum_{\ell=1}^{n}p(\beta_\ell)\right) \\ && \times|_i<0|\sigma^+(0,0)|\beta_n,\cdots,\beta_1>_{\epsilon_n,\dots,\epsilon_1;i}|^2 \\ && \times\left(1+\exp\left(i\left(k+\sum_{\ell=1}^{n}p(\beta_\ell)\right)\right)\right) \\ &\to& \epsilon^n C_{3,n}\sum'_{\epsilon_1,\cdots,\epsilon_n}d\beta_1\cdots\int_{-\infty}^{+\infty}d\beta_n \\ && \times\delta\left(w-\sum_{\ell=1}^{n}e(\beta_\ell)\right)\delta\left(k+\sum_{\ell=1}^{n}p(\beta_\ell)\right) \\ && \times|_i<0|\sigma^+(0,0)|\beta_n,\cdots,\beta_1>_{\epsilon_n,\dots,\epsilon_1;i}|^2,\end{array} \tag{30}$$

with

$$C_{3,n}=2n\pi^2C_{2,n}=2^{1-n}\pi^{2(1-n)}((n-1)!)^{-1}. \tag{31}$$

From the expression of the form factor as given by (18) it is clear that it has simple poles coming from the $\Gamma(z)$ function. As shown in Figure 1. the contours $\bar{C}_b$ enclose the simple poles $\beta_{\ell_b}+\frac{\pi i}{2}-2s_{\ell_b}\pi i$ with $1\leq\ell_b\leq n$ and $s_{\ell_b}\in N$, i.e., any nonnegative integer. In Figure 1. these poles are represented by the cross x and not the disk. The contours $\bar{C}_b$ enclose also all the points denoted by the cross x with negative s_{ℓ_b} but these are not poles of the integrand because the latter is analytic at these points and therefore their contribution to the integral is zero. For this

purpose let us recall that the $\Gamma(z)$ function is analytic everywhere on the complex plane except at the negative integer simple poles $z=-s$, with residues given by :

$$Res_{z=-s}\Gamma(z) = \frac{(-1)^s}{s!}, \quad s \geq 0. \tag{32}$$

Consequently, we can explicitly perform the complex integration of the form factor with respect to the integration variables α_b in (18). Indeed, using the following relations :

$$\begin{array}{rcl} \sinh(\beta+\frac{\pi i}{2}-2\pi i s) &=& i\cosh(\beta), \\ \Gamma(-i\beta-s) &=& \frac{(-1)^s\pi i}{\Gamma(i\beta+s+1)\sinh(\pi\beta)}, \\ \Gamma(s+1) &=& s!, \end{array} \tag{33}$$

with s being any non-negative integer and β any real variable, we find :

$$\begin{array}{l} {}_i\!< 0|\sigma^+(0,0)|\beta_n,\ldots,\beta_1>_{-,\ldots,\epsilon_{b_N},\ldots,-,\ldots,\epsilon_{b_1},\ldots,-;i} \sim \epsilon^{-n/2} C^{b_N,\ldots,b_1}_{4,i,n} f(\beta_1,\ldots,\beta_n) \\ \quad \times \sum_{\ell_N,\ldots,\ell_1=1}^n \sum_{s_N,\ldots,s_1=0}^\infty D^{s_N,\ldots,s_1}_{b_N,\ldots,b_1;\ell_N,\ldots,\ell_1}(\beta_1,\ldots,\beta_n) H^{s_N,\ldots,s_1}_{\ell_N,\ldots,\ell_1}(\beta_1,\ldots,\beta_n), \\ \sum_{1=b_1<b_2<\cdots<b_N}^n |_i < 0|\sigma^+(0,0)|\beta_n,\cdots,\beta_1>_{-,\ldots,\epsilon_{b_N},\ldots,-,\ldots,\epsilon_{b_1},\ldots,-;i}|^2 \sim \epsilon^{-n} C_{5,n} F(\beta_1,\cdots,\beta_n) \\ \quad \times \sum_{\ell_{2N},\ldots,\ell_1=1}^n \sum_{s_{2N},\ldots,s_1=0}^\infty S^{s_{2N},\ldots,s_1}_{\ell_{2N},\ldots,\ell_1}(\beta_1,\cdots,\beta_n), \end{array} \tag{34}$$

where again the infinitesimal ϵ is defined by (17) and :

$$\begin{array}{rcl} H^{s_N,\ldots,s_1}_{\ell_N,\ldots,\ell_1}(\beta_1,\ldots,\beta_n) &=& \prod_{a=1}^N \cosh(\beta_{\ell_a})\gamma(s_a)\prod_{a'>a}^N \cosh(\pi\rho_{\ell_a\ell_{a'}}) \\ && \times\prod_{a=1}^N \prod_{1=n_a\neq\ell_1,\ldots,\ell_a}^n \frac{1}{\sinh(\pi\rho_{\ell_a n_a})}\prod_{1=m_a\neq\ell_a}^n \gamma(s_a+i\rho_{\ell_a,m_a}), \\ D^{s_{N+c},\ldots,s_{1+c}}_{b_N,\ldots,b_1;\ell_{N+c},\ldots,\ell_{1+c}}(\beta_1,\ldots,\beta_n) &=& \prod_{a=1+c}^{N+c}\prod_{a'>a}^{N+c}(i\rho_{\ell_a\ell_{a'}}+s_a-s_{a'}-\frac{1}{2}) \\ && \times\prod_{1=m_a\neq b_a}^n (s_a+i\rho_{\ell_a m_a}-\frac{\Theta(b_{a-c}-m_a)}{2}) \\ L^{s_{2N},\ldots,s_1}_{\ell_{2N},\ldots,\ell_1}(\beta_1,\ldots,\beta_n) &=& \sum_{1=b_1<b_2<\cdots<b_N}^n D^{s_{2N},\ldots,s_{N+1}}_{b_N,\ldots,b_1;\ell_{2N},\ldots,\ell_{N+1}}(\beta_1,\ldots,\beta_n) \\ && \times D^{s_N,\ldots,s_1}_{b_N,\ldots,b_1;\ell_N,\ldots,\ell_1}(\beta_1,\ldots,\beta_n)^*, \\ S^{s_{2N},\ldots,s_1}_{\ell_{2N},\ldots,\ell_1}(\beta_1,\cdots,\beta_n) &=& H^{s_{2N},\ldots,s_{N+1}}_{\ell_{2N},\ldots,\ell_{N+1}}(\beta_1,\ldots,\beta_n) L^{s_{2N},\ldots,s_1}_{\ell_{2N},\ldots,\ell_1}(\beta_1,\ldots,\beta_n) H^{s_N,\ldots,s_1}_{\ell_N,\ldots,\ell_1}(\beta_1,\ldots,\beta_n)^*, \\ f(\beta_1,\ldots,\beta_n) &=& \prod_{\ell>\ell'=1}^n \frac{A_-(2\pi\rho_{\ell\ell'})}{A_-(\pi i/2)\Gamma(1/4)}\prod_{\ell=1}^n \frac{\pi i}{\sinh(\pi i/4-\beta_\ell/2)}, \\ F(\beta_1,\ldots,\beta_n) &=& \frac{\prod_{\ell>\ell'=1}^n A(2\pi\rho_{\ell\ell'})}{\prod_{\ell=1}^n \cosh(\beta_\ell)}, \\ C^{b_N,\ldots,b_1}_{4,i,n} &=& i^{(n-2)(11n-20)/8+2\sum_{a=1}^N b_a} 2^{(n-2)(6n-8)/8}\pi^{(n-2)(9n-8)/8} C_{1,i,n} \\ &=& i^{(13n^2-34n+40)/8-2i+2\sum_{a=1}^N b_a} 2^{2(1-n)}\pi^{(n-2)^2/4}\Gamma(3/4)^{-n/2} A_+(\pi i/2)^{-n/2}, \\ C_{5,n} &=& |C_{4,i,n}|^2 (2\pi^2)^n \Gamma(1/4)^{-n(n-1)}|A_-(\pi i/2)|^{-n(n-1)} \\ &=& 2^{(n^2-38n+48)/12}\pi^2 e^{n(n-2)/4} A^{-3n(n-2)}, \\ c &=& 0, N; \\ \ell_a &=& 1,\cdots,n; \quad a=1,\cdots,2N \\ s_a &=& 0,1,\cdots,\infty, \quad a=1,\cdots,2N. \end{array} \tag{35}$$

Here N is defined by (19) and $\Theta(x)$ is the usual Heaviside step function defined as $\Theta(x)=0$ for $x\leq 0$ and $\Theta(x)=1$ for $x>1$. Furthermore, we have used relations (21) and introduced the notations :

$$\begin{array}{rcl} \rho_{ab} &\equiv& \frac{\beta_a-\beta_b}{2\pi}, \\ \gamma(z) &\equiv& \frac{\Gamma(z-\frac{1}{2})}{\Gamma(z+1)}. \end{array} \tag{36}$$

Given the latter we can easily check that for any non-negative integer s we have

$$\begin{array}{rcl} \gamma(s) &=& \frac{(2s-2)!}{2^{2s-2}s!(s-1)!}\sqrt{\pi}, \quad s\geq 1, \\ \gamma(0) &=& -2\sqrt{\pi}. \end{array} \tag{37}$$

Also note the fact that the $A_-(\beta)$ function is an even function with respect to the permutation of the spectral parameters β_1 and β_2, i.e.,

$$A_-(2\pi\rho_{ab}) = A_-(-2\pi\rho_{ab}) = A_-(2\pi\rho_{ba}). \tag{38}$$

To optimize the numerical evaluations of the DSF it is worth expressing the functions $\Gamma(z-s+1)$ for any non-negative s in terms of the function $\Gamma(z+1)$ without s and the Pochhammer symbol $(z)_s$ defined as :

$$\begin{array}{rcl} (z)_s & = & z(z-1)\dots(z-s+1) = \frac{\Gamma(z+1)}{\Gamma(z-s+1)}, \quad s \geq 1, \\ (z)_0 & = & 1. \end{array} \tag{39}$$

Substituting relation (34) back in (30) we find that the n-spinon DSF can be written in terms of $S^{s_{2N},\dots,s_1}_{\ell_{2N},\dots,\ell_1}(\beta_1,\cdots,\beta_n)$ function as :

$$\begin{array}{rcl} S^{i,+-}_n(w,k-\pi) & = & C_{6,n}\int_{-\infty}^{+\infty} d\beta_1 \cdots \int_{-\infty}^{+\infty} d\beta_n \\ & & \times\delta\left(k+\sum_{\ell=1}^n p(\beta_\ell)\right) \\ & & \times\delta\left(w-\sum_{\ell=1}^n e(\beta_\ell)\right) \\ & & \times F(\beta_1,\cdots,\beta_n) \\ & & \times\sum_{\ell_{2N},\dots,\ell_1=1}^n \sum_{s_{2N},\dots,s_1=0}^\infty S^{s_{2N},\dots,s_1}_{\ell_{2N},\dots,\ell_1}(\beta_1,\cdots,\beta_n), \end{array} \tag{40}$$

with

$$C_{6,n} = C_{3,n}C_{5,n} = n2^{(n^2-50n+60)/12}\pi^{2(2-n)}(n!)^{-1}e^{n(n-2)/4}A^{-3n(n-2)}. \tag{41}$$

Integrating the two delta functions over β_1 and β_2 we obtain :

$$\begin{array}{rcl} S^{i,+-}_n(w,k-\pi) & = & C_{6,n}\int_{-\infty}^{+\infty} d\beta_3 \cdots \int_{-\infty}^{+\infty} d\beta_n \\ & & \sum_{(\bar\beta_1,\bar\beta_2,\beta_3,\cdots,\beta_n)\in E} \\ & & \times\frac{\bar F(\bar\beta_1,\bar\beta_2,\beta_3,\cdots,\beta_n)\Theta(W_u-W)\Theta(W-W_l)}{\sqrt{W_u^2-W^2}} \\ & & \times\sum_{\ell_{2N},\dots,\ell_1=1}^n \sum_{s_{2N},\dots,s_1=0}^\infty S^{s_{2N},\dots,s_1}_{\ell_{2N},\dots,\ell_1}(\bar\beta_1,\bar\beta_2,\beta_3,\cdots,\beta_n), \end{array} \tag{42}$$

where

$$\begin{array}{rcl} \bar F(\bar\beta_1,\bar\beta_2,\beta_3,\cdots,\beta_n) & = & \cosh(\bar\beta_1)\cosh(\bar\beta_2)F(\bar\beta_1,\bar\beta_2,\beta_3,\cdots,\beta_n) = \frac{\prod_{m>\ell=1}^n A(2\pi\rho_{m\ell})}{\prod_{\ell=3}^n \cosh(\beta_\ell)}, \\ W & = & e(\bar\beta_1)+e(\bar\beta_2) = w-\sum_{\ell=3}^n e(\beta_\ell) = w-\pi\sum_{\ell=3}^n \frac{1}{\cosh(\beta_\ell)}, \\ K & = & -p(\bar\beta_1)-p(\bar\beta_2) = k+\sum_{\ell=3}^n p(\beta_\ell) = k+\sum_{\ell=3}^n \operatorname{arccot}(\sinh(\beta_\ell)), \\ W_u & = & 2\pi|\sin(K/2)|, \\ W_l & = & pi|\sin(K)|, \\ \bar\beta_1 & = & \operatorname{arcsinh}\left(\cot\left(-\frac{K}{2}+\arccos(\frac{W}{W_u})\right)\right), \\ \bar\beta_2 & = & \operatorname{arcsinh}\left(\cot\left(-\frac{K}{2}-\arccos(\frac{W}{W_u})\right)\right), \end{array} \tag{43}$$

and E is the set of all $(\bar\beta_1,\bar\beta_2,\beta_3,\cdots,\beta_n)$ that satify the latter relations for fixed k and w. This set is generated from the actions of the permutation elements P_{12} and $P_{ij}, i\neq 1,2; j\neq 1,2; i\neq j$ on the natuarally ordered set $(\bar\beta_1,\bar\beta_2,\beta_3,\cdots,\beta_n)$. This means $dim(E) = 2\times(n-2)!$. To show that all the elements of E contribute the same value to the integral one can easily check that the

following identities hold true :

$$
\begin{array}{rcl}
X^{s_{2N},\dots,s_1}_{\ell_{2N},\dots,\ell_1}(\beta_1,\cdots,\beta_n) &=& X^{s_N,\dots,s_1,s_{2N},\dots,s_{N+1}}_{\ell_N,\dots,\ell_1,\ell_{2N},\dots,\ell_{N+1}}(\beta_1,\cdots,\beta_n)^*, \\
X^{s_N,\dots,s_1,s_N,\dots,s_1}_{\ell_N,\dots,\ell_1,\ell_N,\dots,\ell_1}(\beta_1,\cdots,\beta_n) &=& X^{s_N,\dots,s_1,s_N,\dots,s_1}_{\ell_N,\dots,\ell_1,\ell_N,\dots,\ell_1}(\beta_1,\cdots,\beta_n)^* \in R, \\
H^{s_N,\dots,s_1}_{\ell_N,\cdots,\ell_b,\cdots,\ell_a,\cdots,\ell_1,P_{a,b}}(\beta_1,\cdots,\beta_a,\cdots,\beta_b\cdots,\beta_n) &=& H^{s_N,\dots,s_1}_{\ell_N,\cdots,\ell_a,\cdots,\ell_b,\cdots,\ell_1}(\beta_1,\cdots,\beta_a,\cdots,\beta_b\cdots,\beta_n), \\
H^{s_N,\dots,s_1}_{\ell_N,\cdots,\ell_1,P_{c,d}}(\beta_1,\cdots,\beta_c,\cdots,\beta_d\cdots,\beta_n) &=& H^{s_N,\dots,s_1}_{\ell_N,\cdots,\ell_1}(\beta_1,\cdots,\beta_c,\cdots,\beta_d\cdots,\beta_n), \\
&& c\neq \ell_1,\cdots,\ell_N, \quad d\neq \ell_1,\cdots,\ell_N, \\
F_{P_{a,b}}(\beta_1,\beta_2,\cdots,\beta_{n-1},\beta_n) &=& F(\beta_1,\beta_2,\cdots,\beta_{n-1},\beta_n), \quad a,b=1,\cdots,n, \quad a\neq b,
\end{array}
\tag{44}
$$

where for some function $G(\beta_1,\cdots,\beta_n)$ with its arguments ordered in the natual ordering $(\beta_1,\beta_2,\cdots,\beta_{n-1},\beta_n)$ we have introduced the action of the permutation group on its arguments as :

$$
G_{P_{a,b}}(\beta_1,\beta_2,\cdots,\beta_{n-1},\beta_n)=G(\beta_{\tau_{(1)}},\beta_{\tau_{(2)}},\cdots,\beta_{\tau_{(n-1)}},\beta_{\tau_{(n)}}), \tag{45}
$$

with the action of the transposition $P_{a,b}$ operator on the naturally ordered set $(\beta_1,\beta_2,\cdots,\beta_{n-1},\beta_n)$ defined as usual by :

$$
P_{a,b}(\beta_1,\beta_2,\cdots,\beta_{n-1},\beta_n)=(\beta_{\tau_{(1)}},\beta_{\tau_{(2)}},\cdots,\beta_{\tau_{(n-1)}},\beta_{\tau_{(n)}}). \tag{46}
$$

For example

$$
G_{P_{1,3}}(\beta_1,\beta_2,\beta_3,\cdots,\beta_{n-1},\beta_n)=G(\beta_3,\beta_2,\beta_1,\cdots,\beta_{n-1},\beta_n). \tag{47}
$$

In the above identities we denote by $X^{s_{2N},\dots,s_1}_{\ell_{2N},\dots,\ell_1}(\beta_1,\cdots,\beta_n)$ either $L^{s_{2N},\dots,s_1}_{\ell_{2p},\dots,\ell_1}(\beta_1,\cdots,\beta_n)$ or $S^{s_{2N},\dots,s_1}_{\ell_{2N},\dots,\ell_1}(\beta_1,\cdots,\beta_n)$, that is, both of the latter functions satisfy exactly the same identities given by the first two relations in (44). Let us note from the latter identities also that the function $F(\beta_1,\beta_2,\cdots,\beta_{n-1},\beta_n)$ is fully symmetric function under the permutation group acting on all its arguments. Furthermore let us note that the choice of the integration variables β_1,β_2 in (40) was arbitrary and we could have picked any other pair. The number of all possible pairs in $(\beta_1,\beta_2,\cdots,\beta_n)$ is $n\times(n-1)/2$. Because of the latter identities and redefinitions on the integration variables all the elements of the set E contribute equally for a total overall factor of $2\times(n-2)!\times n(n-1)/2=n!$ which is just the multiplicity factor of the energy-momenta conservation laws $k=-\sum_{\ell=1}^n p_\ell$ and $w=\sum_{\ell=1}^n e_\ell$ since there are $n!$ ways to permute the p_ℓ such that all these configurations satisfy the latter laws. The n-spinon DSF $S_n^{i,+-}$ simplifies then to :

$$
\begin{array}{rcl}
S_n^{i,+-}(w,k-\pi) &=& C_{7,n}\int_{-\infty}^{+\infty}d\beta_3\cdots\int_{-\infty}^{+\infty}d\beta_n \\
&& \times\frac{\bar F(\bar\beta_1,\bar\beta_2,\beta_3,\cdots,\beta_n)\Theta(W_u-W)\Theta(W-W_l)}{\sqrt{W_u^2-W^2}} \\
&& \times\sum_{\ell_{2N}>=\ell_N,\ell_{2N-1},\dots,\ell_1=1}^{n}\sum_{s_{2N},\dots,s_1=0}^{\infty}(2-\delta_{\ell_{2N}\ell_N})Re(S^{s_{2N},\dots,s_1}_{\ell_{2N},\dots,\ell_1}(\bar\beta_1,\bar\beta_2,\beta_3\cdots,\beta_n)),
\end{array}
\tag{48}
$$

with

$$
C_{7,n}=n!C_{6,n}=n2^{(n^2-50n+60)/12}\pi^{2(2-n)}e^{n(n-2)/4}A^{-3n(n-2)}. \tag{49}
$$

Note that in general the overall factor $C_{7,n}$ is simply expressed in terms of the Glaisher-Kinkelin constant A. This is a new result as far as the author knows. Note also that $C_{7,2}=1/4$ which is also is a new result that was previously unknown albeit this value was first used without any proof or justification in reference [18] (to bre more precise the latter reference used a value of $1/2$ which is double the correct value due to the inclusion of both sectors i which was also incorrect as we will see shortly in the sequel). Since $S_n^{i,+-}$ is independent of the sector index i we have decided to omit any reference to it in the sequel. This also means that both sectors contribute equally and we just need to focus on one of them. In fact we will prove next that only one sector leads to the full physical DSF. In the initial paper [16] a mistake was made by adding

up the contributions from both ssectors to get the physical DSF which in turn made the overall normalization factor overvalued by a factor of 2. Let us now prove why it was incorrect to do so in this initial paper [16]. For this purpose let us integrate both sides of the total $S^i(w,k)$ as given by relation (8) with respect to both w and k :

$$\begin{array}{rcl} \frac{1}{(2\pi)^2}\int_0^\infty dw \int_{-\pi}^{\pi} dk S^{i,+-}(w,k) & = & \frac{1}{(2\pi)^2}\int_0^{2\pi} dw \int_{-\pi}^{\pi} dk \int_{-\infty}^{\infty} dt \sum_{n\in Z} e^{i(wt+kn)} \\ & & \times_i < 0|\sigma^+(t,n)\sigma^-(0,0)|0>_i \\ & = & \int_{-\infty}^{\infty} dt \sum_{n\in Z} \delta(t)\delta(n) < 0|\sigma^+(t,n)\sigma^-(0,0)|0>_i \\ & = & {}_i < 0|\sigma^+(0,0)\sigma^-(0,0)|0>_i = \frac{1}{2}, \end{array} \tag{50}$$

with

$$\sigma^+(0,0)\sigma^-(0,0) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}(0,0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}(0,0). \tag{51}$$

This is an extremely important result known in the litterature as the total integrated intensity sum rule. Also the value 1/2 is the well known full physical value of the static one point function of the local operator ${}_i < 0|\sigma^+(0,0)\sigma^-(0,0)|0>_i$. The crucial point to note here is that it is obtained from just from one sector i without summation over both sectors i and is indeed independent of i as was calculated in both references [22] and [13]. Since the full physical static one point fonction is a limiting particular case of the dynamic full physical DSF and is obtained from just one sector this means the latter must also be obtained from just one sector. Since it should not depend on which one of the two possible sectors $i = 0, 1$ the latter two must therefore contribute equally, or put otherwise, the DSF should be independent of i. Given that the full physical DSF is the sum of the n-spinon DSF $S_n^{i,+-}$ the latter is also the full physical one and should also be independent of i which is indeed the case as shown by (48). This should be expected because recall that i fixes the boundary conditions such that the allowable spin configurations are those for which the eigenvalues of σ_n^z are $(-1)^{i+n}$ in the limit $n \to \pm\infty$. So the two eigenspaces corresponding to the two sectors are completely disjoint and it would take an infinite energy to jump from one state from one sector to another state in the other sector. Therefore there can be no interference between the two eigenspaces and the physical DSF is built on any one ot them but not the two at the same time. This concludes the proof that we should not sum up the contributions of the 2 sectors $i = 0, 1$ to get the physical n-spinon DSF.

2.1 2-spinon DSF

This case is characterized by $n = 2$ and empty set B for the only allowed configuration $(\epsilon_2, \epsilon_1) = (-,-)$ and therefore the general formulas (18) and (35) simplify considerably to :

$$\begin{array}{rcl} & & {}_i< 0|\sigma^+(0,0)|\xi_2,\xi_1 >_{--;i} \\ & \to & {}_i< 0|\sigma^+(0,0)|\beta_2,\beta_1 >_{--;i} \\ & \to & -_{1-i}< 0|\sigma^+(0,0)|\beta_2,\beta_1 >_{--;1-i} \\ & \sim & \epsilon^{-1} C_{1,i,2} \frac{A_-(\beta_2-\beta_1)}{A_-(\pi i/2)\Gamma(1/4)} \prod_{\ell=1}^{2} \frac{\pi i}{\sinh(\pi i/4-\beta_\ell/2)} \\ & & |_i < 0|\sigma^+(0,0)|\xi_n,\xi_1 >_{--;i}|^2 \\ & \to & |_i < 0|\sigma^+(0,0)|\beta_2,\beta_1 >_{--;i}|^2 \\ & \sim & \epsilon^{-2} C_{5,2} A(\beta_2-\beta_1) \\ C_{1,i,2} & = & -i^{1-2i} 2^{-2}\Gamma(3/4)^{-1} A_+(\pi i/2)^{-1}, \\ C_{5,2} & = & 2^{-2}\pi^2, \\ p(\xi_\ell) & \to & p(\beta_\ell), \quad \cot(p(\beta_\ell)) = \sinh(\beta_\ell), \quad -\pi \le p(\beta_\ell) \le 0, \\ e(\xi_\ell) & \to & e(\beta_\ell) = \frac{\pi}{\cosh(\beta_\ell)} = -\pi\sin(p(\beta_\ell)), \quad 0 \le e(\beta_\ell) \le \pi, \quad 1 \le \ell \le 2, \\ \oint \frac{d\xi_1}{2\pi i\xi_1}\oint \frac{d\xi_2}{2\pi i\xi_2} & \to & \epsilon^2 2^{-2}\pi^{-4}\int_{-\infty}^{+\infty} d\beta_1 \int_{-\infty}^{+\infty} d\beta_2. \end{array} \tag{52}$$

Because of the latter simple relations the general formula of n-spinon S_n^{+-} (48) simplifies substantially as well to :

$$S_2^{+-}(w,k-\pi)=\frac{1}{4}\frac{A(\bar{\beta}_2-\bar{\beta}_1)\Theta(W_u-w)\Theta(w-W_l)}{\sqrt{W_u^2-w^2}}, \tag{53}$$

where

$$\begin{array}{rcl} W & = & w=e(\bar{\beta}_1)+e(\beta_2), \quad 0\le w\le 2\pi, \\ K & = & k=-p(\bar{\beta}_1)-p(\bar{\beta}_2), \quad 0\le k\le 2\pi, \\ W_u & = & 2\pi\sin(k/2), \\ W_l & = & \pi|\sin(k)|, \\ \bar{\beta}_1(w,k) & = & \operatorname{arcsinh}\left(\cot\left(-\frac{k}{2}+\arccos(\frac{w}{W_u})\right)\right), \\ \bar{\beta}_2(w,k) & = & \operatorname{arcsinh}\left(\cot\left(-\frac{k}{2}-\arccos(\frac{w}{W_u})\right)\right). \end{array} \tag{54}$$

Plotting the dispersion relation of w as a function of k in Figure 2 we can see that w lies between two boundaries. The upper boundary is given by W_u and the lower boundary is given by W_l which is also known as des Cloizeaux-Pearson dispersion relation. For the sake of comparison with experimental data where the DSF is given for the local spins normalized as :

$$S^x=\frac{1}{2}\begin{pmatrix}0&1\\1&0\end{pmatrix}, \qquad S^y=\frac{1}{2}\begin{pmatrix}0&-i\\i&0\end{pmatrix}, \qquad S^z=\frac{1}{2}\begin{pmatrix}1&0\\0&-1\end{pmatrix}, \tag{55}$$

we consider then the following nonvanishing components of the 2-spinon DSF :

$$S_2^{xx}(w,k-\pi)=S_2^{yy}(w,k-\pi)=S_2^{zz}(w,k-\pi)=\frac{1}{2}S_2^{+-}(w,k-\pi). \tag{56}$$

The latter components are equal because of the isotropy of the Heisenberg model. In Figure 3 we plot S_2^{zz} as a function of w for fixed $k=\pi$. Note from relation (53) despite the presence of the term $\sqrt{W_u^2-w^2}$ in the denominator of S_2^{zz} the latter actually vanishes at this boundary. This is physically expected because this boundary is characterized by equal momenta of the 2 spinons (i.e., equal spectral parameters $\bar{\beta}_1$ and $\bar{\beta}_2$ as can be seen from (54)). Since the two spinons are fermions in nature and they have the same spin therefore they cannot have equal momenta due to the Pauli exclusion principle for fermions thus leading to vanishing DSF. To see that the upper boundary corresponds to equal spectral parameters $\bar{\beta}_1$ and $\bar{\beta}_2$ it is clear from relations (54) $\bar{\beta}_1(w,k)=\bar{\beta}_2(w,k)$ if

$$\arccos(\frac{w}{W_u})=0, \tag{57}$$

that is :

$$w=W_u. \tag{58}$$

By analogy note from Figure 3 that at the other extreme lower boundary W_l S_2^{zz} diverges leading to a resonnance. This is also physically expected because this boundary is characterized by one momentum being equal to π and the other one being equal to 0, that is, the two spinons which have equal spins are at their maximum difference through the momenta leading to an extreme opposite of the Pauli exclusion principle and which we call the inclusion principle for fermions when they are at their maximum difference, that is, fermions tend to favor being at states where they differ by a maximum amount. This is analogous to bosons which favor being at states which have have exactly equal quantum numbers. Between these two extremes S_2^{zz} takes on non-zero finite values which correspond to the two spinons having equal spins but different momenta that differ by an amount between 0 and π exclusive. The transition between the latter three regimes is a smooth one.

2.2 4-spinon DSF

This case is characterized by $n = 4$ and dim(B) $= 1$ meaning that there are four allowed configurations $(\epsilon_4, \epsilon_3, \epsilon_2, \epsilon_1)$ with all $\epsilon_\ell = -, \ell = 1, 2, 3, 4$ except one of them being equal to $+$. The general formulas in (18) take the following considerably simpler form :

$$\begin{array}{rcl} & & {}_i\!< 0|\sigma^+(0,0)|\xi_4, ..., \xi_1 >_{-,\ldots,\epsilon_b,\ldots,-;i} \\ & \to & {}_i\!< 0|\sigma^+(0,0)|\beta_4, ..., \beta_1 >_{-,\ldots,\epsilon_b,\ldots,-;i} \\ & \to & -_{1-i}\!< 0|\sigma^+(0,0)|\beta_4, ..., \beta_1 >_{-,\ldots,\epsilon_b,\ldots,-;1-i} \\ & \sim & \epsilon^{-2} C_{1,i,4} \\ & & \times \prod_{m>\ell=1}^{4} \frac{A_-(\beta_m-\beta_\ell)}{A_-(\pi i/2)\Gamma(1/4)} \prod_{\ell=1}^{4} \frac{\pi i}{\sinh(\pi i/4-\beta_\ell/2)} \\ & & \times \int_{\bar{C}_b} \frac{d\alpha_b}{2\pi i} \sinh(\alpha_b) \\ & & \times \prod_{\ell=1}^{b-1}(\alpha_b - \beta_\ell + \frac{\pi i}{2}) \prod_{\ell=b+1}^{4}(\beta_\ell - \alpha_b + \frac{\pi i}{2}) \\ & & \times \prod_{\ell=1}^{4} \Gamma(-\frac{1}{4} + \frac{\alpha_b-\beta_\ell}{2\pi i})\Gamma(-\frac{1}{4} - \frac{\alpha_b-\beta_\ell}{2\pi i}) \\ C_{1,i,4} & = & (-1)^i 2^{-10}\pi^{-6}\Gamma(3/4)^{-2}A_+(\pi i/2)^{-2}, \\ p(\xi_\ell) & \to & p(\beta_\ell), \quad \cot(p(\beta_\ell)) = \sinh(\beta_\ell), \quad -\pi \le p(\beta_\ell) \le 0, \\ e(\xi_\ell) & \to & e(\beta_\ell) = \frac{\pi}{\cosh(\beta_\ell)} = -\pi\sin(p(\beta_\ell)), \quad 0 \le e(\beta_\ell) \le \pi, \quad 1 \le \ell \le 4, \\ \oint \frac{d\xi_1}{2\pi i\xi_1} ... \oint \frac{d\xi_n}{2\pi i\xi_4} & \to & \epsilon^4 2^{-4}\pi^{-8} \int_{-\infty}^{+\infty} d\beta_1 ... \int_{-\infty}^{+\infty} d\beta_4, \\ & & \epsilon_b = +, \quad b = 1, \cdots, 4 \end{array} \tag{59}$$

The infinitesimal ϵ is defined by (17) and the single contour $\bar{C}_b$ is displayed in Figure 1. Moreover, the general relations (34) and (35) become for $n = 4$:

$$\begin{array}{rcl} {}_i\!< 0|\sigma^+(0,0)|\beta_4, \ldots, \beta_1 >_{-,\ldots,\epsilon_b,\ldots,-;i} & \sim & \epsilon^{-2} C^b_{4,i,4} f(\beta_1, \ldots, \beta_4) \\ & & \times \sum_{\ell=1}^{4} \sum_{s=0}^{\infty} D^s_{b;\ell}(\beta_1, \ldots, \beta_4) H^s_\ell(\beta_1, \ldots, \beta_4), \\ \sum_{b=1}^{4} |{}_i < 0|\sigma^+(0,0)|\beta_4, \cdots, \beta_1 >_{-,\ldots,\epsilon_b,\ldots,-;i}|^2 & \sim & \epsilon^{-4} C_{5,4} F(\beta_1, \cdots, \beta_4) \\ & & \times \sum_{\ell_2,\ell_1=1}^{4} \sum_{s_2,s_1=0}^{\infty} S^{s_2,s_1}_{\ell_2,\ell_1}(\beta_1, \cdots, \beta_4), \end{array} \tag{60}$$

where :

$$\begin{array}{rcl} H^s_\ell(\beta_1, \ldots, \beta_4) & = & \cosh(\beta_\ell)\gamma(s) \prod_{1=m\neq\ell}^{4} \frac{\gamma(s+i\rho_{\ell,m})}{\sinh(\pi\rho_{\ell m})}, \\ D^s_{b;\ell}(\beta_1, \ldots, \beta_4) & = & \prod_{1=m\neq b}^{4}(s + i\rho_{\ell m} - \Theta(b-m)/2) \\ L^{s_2,s_1}_{\ell_2,\ell_1}(\beta_1, \ldots, \beta_4) & = & \sum_{b=1}^{4} D^{s_2}_{b;\ell_2}(\beta_1, \ldots, \beta_4) D^{s_1}_{b;\ell_1}(\beta_1, \ldots, \beta_4)^*, \\ S^{s_2,s_1}_{\ell_2,\ell_1}(\beta_1, \cdots, \beta_4) & = & H^{s_2}_{\ell_2}(\beta_1, \ldots, \beta_4) L^{s_2,s_1}_{\ell_2,\ell_1}(\beta_1, \ldots, \beta_4) H^{s_1}_{\ell_1}(\beta_1, \ldots, \beta_4)^*, \\ f(\beta_1, \ldots, \beta_4) & = & \prod_{\ell>\ell'=1}^{4} \frac{A_-(2\pi\rho_{\ell\ell'})}{A_-(\pi i/2)\Gamma(1/4)} \prod_{\ell=1}^{4} \frac{\pi i}{\sinh(\pi i/4-\beta_\ell/2)}, \\ F(\beta_1, \ldots, \beta_4) & = & \frac{\prod_{\ell>\ell'=1}^{4} A(2\pi\rho_{\ell\ell'})}{\prod_{\ell=1}^{4}\cosh(\beta_\ell)}, \\ C^b_{4,i,4} & = & (-1)^{1+b-i} 2^{-6}\pi\Gamma(3/4)^{-2}A_+(\pi i/2)^{-2}, \\ C_{5,4} & = & 2^{-22/3}\pi^2 e^2 A^{-24} \\ \ell_1, \ell_2 & = & 1, \cdots, 4; \\ s_1, s_2 & = & 0, 1, \cdots, \infty. \end{array} \tag{61}$$

Finally setting $n = 4$ in the general expression (48) of S^{+-}_n we obtain :

$$\begin{array}{rcl} S^{i,+-}_4(w, k-\pi) & = & C_{7,4} \int_{-\infty}^{+\infty} d\beta_3 \int_{-\infty}^{+\infty} d\beta_4 \\ & & \times \frac{\bar{F}(\bar{\beta}_1,\bar{\beta}_2,\beta_3,\cdots,\beta_6)\Theta(W_u-W)\Theta(W-W_l)}{\sqrt{W_u^2-W^2}} \\ & & \times \left(\sum_{\ell_4>=\ell_2,\ell_3,\ell_1=1}^{4} \sum_{s_4,s_3,s_2,s_1=0}^{\infty} (2-\delta_{\ell_4\ell_2}) Re(S^{s_4,s_3,s_2,s_1}_{\ell_4,\ell_3,\ell_2,\ell_1}(\bar{\beta}_1, \bar{\beta}_2, \beta_3, \beta_4))\right), \end{array} \tag{62}$$

where

$$
\begin{array}{rcl}
\bar{F}(\bar{\beta}_1,\bar{\beta}_2,\beta_3,\beta_4) &=& \cosh(\bar{\beta}_1)\cosh(\bar{\beta}_2)F(\bar{\beta}_1,\bar{\beta}_2,\beta_3,\beta_4) = \frac{\prod_{b>a=1}^{4} A(2\pi\rho_{ba})}{\cosh(\beta_3)\cosh(\beta_4)},\\
W &=& e(\bar{\beta}_1)+e(\bar{\beta}_2) = w-e(\beta_3)-e(\beta_4) = w-\pi\frac{\cosh(\beta_3)+\cosh(\beta_4)}{\cosh(\beta_3)\cosh(\beta_4)},\\
K &=& -p(\bar{\beta}_1)-p(\bar{\beta}_2) = k+p(\beta_3)+p(\beta_4) = k+\mathrm{arccot}(\sinh(\beta_3))+\mathrm{arccot}(\sinh(\beta_4)),\\
W_u &=& 2\pi|\sin(K/2)|,\\
W_l &=& \pi|\sin(K)|,\\
\bar{\beta}_1 &=& \mathrm{arcsinh}\left(\cot\left(-\frac{K}{2}+\arccos(\frac{W}{W_u})\right)\right),\\
\bar{\beta}_2 &=& \mathrm{arcsinh}\left(\cot\left(-\frac{K}{2}-\arccos(\frac{W}{W_u})\right)\right),\\
C_{7,4} &=& 2^{-25/3}\pi^{-4}e^2A^{-24}.
\end{array}
\tag{63}
$$

Note that just in this particular case of $n=4$ new symmetries embodied by new identities arise. Indeed, in addition to the relations (44) satisfied by the matrix functions $X^{s,t}_{\ell,m}(\beta_1,\ldots,\beta_4)$, the vector functions $H^s_\ell(\beta_1,\ldots,\beta_4)$, and the scalar function $F(\beta_1,\ldots,\beta_4)$ which are given by :

$$
\begin{array}{rcl}
X^{s,t}_{\ell,m}(\beta_1,\beta_2,\beta_3,\beta_4) &=& X^{t,s}_{m,\ell}(\beta_1,\beta_2,\beta_3,\beta_4)^*,\\
X^{s,s}_{\ell,\ell}(\beta_1,\beta_2,\beta_3,\beta_4) &=& X^{s,s}_{\ell,\ell}(\beta_1,\beta_2,\beta_3,\beta_4)^* \in R,\\
H^s_{\ell\,P_{\ell,m}}(\ldots,\beta_\ell,\ldots,\beta_m,\ldots) &=& H^s_m(\ldots,\beta_\ell,\ldots,\beta_m,\ldots), \quad \ell\neq m,\\
H^s_{\ell\,P_{m,m'}}(\ldots,\beta_m,\ldots,\beta_{m'},\ldots) &=& H^s_\ell(\ldots,\beta_m,\ldots,\beta_{m'},\ldots), \quad m\neq\ell, \quad m'\neq\ell, \quad m\neq m',\\
F_{P_{\ell,m}}(\beta_1,\beta_2,\beta_3,\beta_4) &=& F(\beta_1,\beta_2,\beta_3,\beta_4), \quad \ell\neq m,\\
&& \ell,m=1,\cdots,4, \quad s,t=0,\cdots,\infty
\end{array}
\tag{64}
$$

we also have the following extra identities satisfied by both matrix functions $X^{s,t}_{\ell,m}(\beta_1,\ldots,\beta_4)=L^{s,t}_{\ell,m}(\beta_1,\ldots,\beta_4)$ and $X^{s,t}_{\ell,m}(\beta_1,\ldots,\beta_4)=S^{s,t}_{\ell,m}(\beta_1,\ldots,\beta_4)$:

$$
\begin{array}{rcl}
X^{s,t}_{\ell,\ell'\,P_{m,m'}}(\beta_1,\beta_2,\beta_3,\beta_4) &=& X^{s,t}_{\ell,\ell'}(\beta_1,\beta_2,\beta_3,\beta_4), \quad \ell\neq m,\ \ell\neq m',\ \ell'\neq m,\ \ell'\neq m',\\
X^{s,t}_{\ell,m\,P_{\ell,m}}(\beta_1,\beta_2,\beta_3,\beta_4) &=& X^{s,t}_{m,\ell}(\beta_1,\beta_2,\beta_3,\beta_4),, \quad \ell\neq m,\\
X^{s,t}_{\ell,\ell\,P_{\ell,m}}(\beta_1,\beta_2,\beta_3,\beta_4) &=& X^{s,t}_{m,m}(\beta_1,\beta_2,\beta_3,\beta_4), \quad \ell\neq m,\\
X^{s,t}_{\ell,\ell'\,P_{\ell,\ell'}P_{\ell',m}}(\beta_1,\beta_2,\beta_3,\beta_4) &=& X^{s,t}_{\ell',m\,P_{\ell',\ell}P_{\ell,m}}(\beta_1,\beta_2,\beta_3,\beta_4) = X^{s,t}_{m,\ell}(\beta_1,\beta_2,\beta_3,\beta_4), \quad \ell\neq\ell',\ \ell\neq m,\ \ell'\neq m,\\
X^{s,t}_{\ell,m}(\ldots,\beta_\ell,\ldots,\beta_m,\ldots) &=& X^{s,t}_{\ell,\ell}(\ldots,\beta_\ell,\ldots,\beta_m,\ldots), \quad if \quad \beta_\ell=\beta_m, \quad \ell\neq m,\\
&& \ell,\ell',m,m'=1,\cdots,4, \quad s,t=0,\cdots,\infty.
\end{array}
\tag{65}
$$

Note that the first relation implies that the functions $X^{s,s}_{\ell,\ell}(\beta_1,\beta_2,\beta_3,\beta_4)$ are real valued for any $\ell=1,\cdots,4$ and non-negative integer s. The most important subset of relations that we will be using in the sequel to simplify even further the expression of 4-spinon S^{+-}_4 (62) is :

$$
\begin{array}{rcl}
S^{s,t}_{\ell,\ell\,P_{\ell,1}}(\beta_1,\beta_2,\beta_3,\beta_4) &=& S^{s,t}_{1,1}(\beta_1,\beta_2,\beta_3,\beta_4), \quad \ell=2,3,4\\
S^{s,t}_{\ell,m\,P_{\ell,1}P_{m,2}}(\beta_1,\beta_2,\beta_3,\beta_4) &=& S^{s,t}_{m,\ell\,P_{m,\ell}P_{\ell,1}P_{m,2}}(\beta_1,\beta_2,\beta_3,\beta_4) = S^{s,t}_{1,2}(\beta_1,\beta_3,\beta_2,\beta_4), \quad 1\leq\ell<m\leq 4.
\end{array}
\tag{66}
$$

The latter two relations express all diagonal terms $S^{s,t}_{\ell,\ell}$ and all off diagnoal terms $S^{s,t}_{\ell,m},(\ell\neq m)$ in terms of the first diagonal term $S^{s,t}_{1,1}$ and the first off diagonal term $S^{s,t}_{1,2}$ respectively. This is the reason that allows us to substantially simplify the 4-spinon DSF to express it only in terms of $S^{s,t}_{1,1}$ and $S^{s,t}_{1,2}$ with $t\geq s$ instead of all possible terms $S^{s,t}_{\ell,m}$ and their complex conjugates. Indeed using the latter relations (66), the invariance of the scalar function $\frac{\bar{F}(\bar{\beta}_1,\bar{\beta}_2,\beta_3,\beta_4)}{\sqrt{W_u^2-W^2}}$ under

the transpositions of $(\bar\beta_1, \bar\beta_2)$, and independently, that of (β_3, β_4), and finally the redefinition of the integration variables from (β_3, β_4) to (β_4, β_3) respectively, we can substantially simplify the 4-spinon DSF (62) to write it in the following form :

$$\begin{aligned} S_4^{+-}(w, k-\pi) = \; & C_{7,4} \sum_{t \geq s=0}^{\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} d\beta_3 d\beta_4 \\ & \times \frac{\bar F(\bar\beta_1, \bar\beta_2, \beta_3, \beta_4)\Theta(W_u - W)\Theta(W - W_l)}{\sqrt{W_u^2 - W^2}} \\ & \times Re\left((2-\delta_{s,t})\left(S_{1,1}^{s,t}(\bar\beta_1, \bar\beta_2, \beta_3, \beta_4)\right.\right. \\ & + S_{1,1}^{s,t}(\bar\beta_2, \bar\beta_1, \beta_3, \beta_4) \\ & \left. + 2S_{1,1}^{s,t}(\beta_3, \bar\beta_1, \bar\beta_2, \beta_4)\right) \\ & + 2\left(S_{1,2}^{s,t}(\bar\beta_1, \bar\beta_2, \beta_3, \beta_4)\right. \\ & + (2-\delta_{s,t}) S_{1,2}^{s,t}(\beta_3, \beta_4, \bar\beta_1, \bar\beta_2) \\ & + 2S_{1,2}^{s,t}(\bar\beta_1, \beta_3, \bar\beta_2, \beta_4) \\ & + 2S_{1,2}^{s,t}(\bar\beta_2, \beta_3, \bar\beta_1, \beta_4) \\ & + (1-\delta_{s,t})\left(S_{1,2}^{s,t}(\bar\beta_2, \bar\beta_1, \beta_3, \beta_4)\right. \\ & + 2S_{1,2}^{s,t}(\beta_3, \bar\beta_1, \bar\beta_2, \beta_4) \\ & \left.\left.\left. + 2S_{1,2}^{s,t}(\beta_3, \bar\beta_2, \bar\beta_1, \beta_4)\right)\right)\right), \end{aligned} \tag{67}$$

which can also be written in a more compact form as :

$$\begin{aligned} S_4^{+-}(w, k-\pi) = \; & C_{7,4} \sum_{t \geq s=0}^{\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} d\beta_3 d\beta_4 \\ & \times \frac{\bar F(\bar\beta_1, \bar\beta_2, \beta_3, \beta_4)\Theta(W_u - W)\Theta(W - W_l)}{\sqrt{W_u^2 - W^2}} \\ & \times \Big(\sum_{P \in Y_{11}} \alpha_{11,P}^{s,t} Re(S_{1,1P}^{s,t}(\bar\beta_1, \bar\beta_2, \beta_3, \beta_4)) \\ & \quad + \sum_{P \in Y_{12}} \alpha_{12,P}^{s,t} Re(S_{1,2P}^{s,t}(\bar\beta_1, \bar\beta_2, \beta_3, \beta_4)) \Big) \end{aligned} \tag{68}$$

with the sets Y_{11} and Y_{12} being subsets of the permutation group acting on $(\bar\beta_1, \bar\beta_2, \beta_3, \beta_4)$ in its natural order, and defined by :

$$\begin{aligned} Y_{11} &= \{1, P_{12}, P_{12}P_{23}\}, \\ Y_{12} &= \{1, P_{12}, P_{13}, P_{23}, P_{13}P_{24}, P_{23}P_{12}, P_{12}P_{23}\}, \end{aligned} \tag{69}$$

and the coefficients given by :

$$\begin{aligned} \alpha_{11,1}^{s,t} &= \alpha_{11,P_{12}}^{s,t} = 2 - \delta_{s,t}, \\ \alpha_{11,P_{12}P_{23}}^{s,t} &= \alpha_{12,P_{13}P_{24}}^{s,t} = 2(2-\delta_{s,t}), \\ \alpha_{12,1}^{s,t} &= 2, \\ \alpha_{12,P_{23}}^{s,t} &= \alpha_{12,P_{23}P_{12}}^{s,t} = 4, \\ 2\alpha_{12,P_{12}}^{s,t} = \alpha_{12,P_{13}}^{s,t} &= \alpha_{12,P_{12}P_{23}}^{s,t} = 4(1-\delta_{s,t}). \end{aligned} \tag{70}$$

As we did in the 2-spinon case we consider the following non-vanishing components of the 4-spinon DSF :

$$S_4^{xx}(w, k-\pi) = S_4^{yy}(w, k-\pi) = S_4^{zz}(w, k-\pi) = \frac{1}{2} S_4^{+-}(w, k-\pi). \tag{71}$$

We plot S_4^{zz} and $S_2^{zz} + S_4^{zz}$ as functions of w for fixed $k = \pi$ in Figures 4 and 5 respectively. As can be seen from Figure 4 S_4^{zz} is non-vanishing in the whole range $[0, 4\pi[$. In particular although very small it is not vanishing in the range $[2\pi, 4\pi[$. The latter fact can be used to detect the presence of 4 spinons experimentally since we know that in the latter range S_2^{zz} is vanishing so any non zaro value of S^{zz} can be interpreted as a sign of the presence of 4 spinons and higher in the spectrum.

3 Sum Rules

Here we will compute the percentage of contribution of S_n^{+-} to the total S^{+-} analytically and numerically in the cases $n = 2, 4$ and only analytically in the general case of $n > 4$. For this purpose we consider the first sum rule satisfied by the total S^{+-}, and which is represented by the following total integrated intensity formula :

$$\int_0^\infty dw \int_0^{2\pi} dk S^{+-}(w, k-\pi) = 2\pi^2. \tag{72}$$

Then we consider the following second sum rule satisfied by the total S^{+-} and which is also known as the first frequency moment at fixed momentum :

$$\int_0^\infty dw w S^{+-}(w, k-\pi) = \frac{16e_0\pi}{3}(1-\cos(k)), \tag{73}$$

with $e_0 = \log(2) - 1/4$. To make analogous arguments and derivations as we will do in the sequel in the case of the first sum rule we rather use the following total integrated form of the second sum rule :

$$\int_0^\infty dw \int_0^{2\pi} dk w S^{+-}(w, k-\pi) = \frac{16e_0\pi}{3}\int_0^{2\pi} dk(1-\cos(k)) = \frac{32e_0\pi^2}{3}. \tag{74}$$

In the sequel we will refer to (72) and (74) as the first sum rule and second sum rule respectively. As we will see below both sum rules involve integrals of S_n^{+-} that are totally symmetric with respect to the permutations of the spectral parameters $\beta_\ell, \ell = 1, \cdots, n$.

3.1 2-spinon

Now we present one of the main results of this paper and that is the contribution of S_2^{+-} to the total S^{+-} is about 36%. For this purpose, let us calculate the contribution of just the 2-spinon DSF to the integral given by the first sum rule (72) with S^{+-} being substituted by S_2^{+-}. For this purpose it is convenient to make a change of variables from (w, k) to $(\bar\beta_1, \bar\beta_2) \equiv (\beta_1, \beta_2)$ given by (54). We expect the integrand to be symmetrical with respect to the permutations of β_1 and β_2. Indeed we have :

$$\begin{aligned}\int_0^\infty dw \int_0^{2\pi} dk S_2^{+-}(w, k-\pi) &= \int_0^{2\pi} dw \int_0^{2\pi} dk S_2^{+-}(w, k-\pi)\\ &= \frac{1}{4}\int_{-\infty}^{+\infty} d\beta_1 \int_{-\infty}^{+\infty} d\beta_2 \frac{A(\beta_2-\beta_1)}{\cosh(\beta_1)\cosh(\beta_2)} = 7.17.\end{aligned} \tag{75}$$

Figure 7 is a plot of the latter integrand as a function of β_1 and β_2. Figure 8 is a also a plot of the latter integrand as a function of β_1 for fixed $\beta_2 = 0$. In both figures we see the manisfestation of the existence of 2 spinons through 2 peaks in the graphs. We remark that in the integral over β_1 and β_2 the term $\Theta(W_u - w)\Theta(w - W_l)$ is always equal to 1 due to relations (54) so it is omitted. But this term allowed us to reduce the integral over w from 0 to infinity to 0 to 2π since the maximum value of W_u is 2π for 2 spinons. This remark holds true for the general case of S_n with obvious changes so it will be understood there as well and we will not be repeating this argument again. If we compare this to the first sum rule (72) we conclude that S_2^{+-} accounts for 36.32% of the total S^{+-}. This is a half of the currently known result in the litterature of 72% as first reported in reference [18]. Again using (54), an analogous calculation considering the second sum rule (74) leads to :

$$\begin{aligned}\int_0^\infty dw \int_0^{2\pi} dk w S_2^{+-}(w, k-\pi) &= \int_0^{2\pi} dw \int_0^{2\pi} dk w S_2^{+-}(w, k-\pi)\\ &= \frac{\pi}{4}\int_{-\infty}^{+\infty} d\beta_1 \int_{-\infty}^{+\infty} d\beta_2 \frac{(\cosh(\beta_1)+\cosh(\beta_2))A(\beta_2-\beta_1)}{\cosh(\beta_1)^2\cosh(\beta_2)^2} = 16.60.\end{aligned} \tag{76}$$

If we compare this result to (74) we come to the conclusion that S_2^{+-} accounts for 35.58% of the total S^{+-}, which confirms the conclusion reached through the first sum rule. As mentioned in the introduction experiemental data obtained in [20] and [21] reveals that the observed contribution accounts roughly only for the third of the total theoretic DSF when the latter was incorrectly believed to be 99%. Since we have just shown that S_2 accounts for 36% which is roughly the third of 100% we believe that a reconcilation between experimental data and theoretical data can be made if the experimental data relates just to the 2-spinon sector.

3.2 4-spinon

In order to evaluate the contribution of $S_4^{+-}(w, k-\pi)$ relative to the total contribution given by the first sum rule (72) it is much convenient to consider the latter in the form

$$\int_0^\infty dw \int_0^{4\pi} dk S^{+-}(w, k-\pi) = 2\int_0^\infty dw \int_0^{2\pi} dk S^{+-}(w, k-\pi) = 4\pi^2, \tag{77}$$

since as we will see below it is much easier to calculate the contribution of S_4^{+-} by considering both w and k in $[0, 4\pi]$. So we substitute S^{+-} by S_4^{+-} as given by (68) in the latter relation, and as we did in the 2-spinon case we make a change of variables from (w, k) to $(\bar{\beta}_1, \bar{\beta}_2) \equiv (\beta_1, \beta_2)$ given by (63). We end up with the following expression :

$$\begin{aligned}
\int_0^\infty dw \int_0^{4\pi} dk S_4^{+-}(w, k-\pi) &= \int_0^{4\pi} dw \int_0^{4\pi} dk S_4^{+-}(w, k-\pi) \\
&= C_{7,4} \sum_{t\geq s=0}^{\infty} \int_{-\infty}^{+\infty} d\beta_1 \cdots \int_{-\infty}^{+\infty} d\beta_4 F(\beta_1, \beta_2, \beta_3, \beta_4) \\
&\quad \times \Big(\sum_{P\in Y_{11}} \alpha_{11,P}^{s,t} Re(S_{1,1\,P}^{s,t}(\beta_1, \beta_2, \beta_3, \beta_4)) \\
&\quad\quad + \sum_{P\in Y_{12}} \alpha_{12,P}^{s,t} Re(S_{1,2\,P}^{s,t}(\beta_1, \beta_2, \beta_3, \beta_4)) \Big) .
\end{aligned} \tag{78}$$

where Y_{11} and Y_{12} are the sets of permutations acting on the four spectral parameters β_ℓ and are defined by (69). The coefficients $\alpha_{11,P}^{s,t}$ and $\alpha_{12,P}^{s,t}$ are given by (70). Using the defining relation (61) of $F(\beta_1, \cdots, \beta_4)$, one can easily check that it is invariant under the permutation group G of the four spectral parameters β_ℓ, that is :

$$F_P(\beta_1, \cdots, \beta_4) = F(\beta_1, \cdots, \beta_4). \tag{79}$$

where P is any permutation acting on the latter parameters. For this reason and because of redefinitions of the latter spectral parameters, the above integrand is fully symmetric under the permutation group G and hence simplifies substantially to :

$$\begin{aligned}
\int_0^\infty dw \int_0^{4\pi} dk S_4^{+-}(w, k-\pi) = &\int_0^{4\pi} dw \int_0^{4\pi} dk S_4^{+-}(w, k-\pi) \\
= &\, C_4 \int_{-\infty}^{+\infty} d\beta_1 ... \int_{-\infty}^{+\infty} d\beta_4 \\
&\times F(\beta_1, \beta_2, \beta_3, \beta_4) \\
&\times \sum_{\ell=1}^{2} \sum_{t\geq s\geq 0}^{\infty} [(3 - 2\delta_{1,\ell})(2 - \delta_{s,t}) \\
&\times Re\left(S_{1,\ell}^{s,t}(\beta_1, \ldots, \beta_4)\right)],
\end{aligned} \tag{80}$$

with

$$C_4 = 4 \times C_{7,4} = 2^{-19/3}\pi^{-4} e^2 A^{-24}. \tag{81}$$

Figure 9 is a plot of one term of the latter integrand with $\ell = 1$ and $s = t = 0$ as a function of β_1 and β_2 for fixed $\beta_3 = 0$ and $\beta_4 = 1$. It shows the manisfestation of 4 spinons in the spectrum through 4 peaks in the graph. With the help of the Genz-Malik algorithm the numeric integration of the latter integral gives :

$$\int_0^\infty dw \int_0^{4\pi} dk S_4^{+-}(w, k-\pi) = 6.98 \pm 0.04. \tag{82}$$

With the first sum rule in its form given by (77), this means that S_4^{+-} contributes $17.68 \pm 0.10\%$ or almost 18% to the total S^{+-}. To make analogous derivations as we did in the case of the first sum rule we use the following form of the second sum rule :

$$\begin{array}{rcl} \int_0^\infty dw \int_0^{4\pi} dkwS^{+-}(w,k-\pi) & = & 2\int_0^\infty dw \int_0^{2\pi} dkwS^{+-}(w,k-\pi) \\ & = & \frac{32e_0\pi}{3}\int_0^{2\pi} dk(1-\cos(k)) = \frac{64e_0\pi^2}{3} \end{array} \tag{83}$$

Now since w as given by (63) is symmetric with respect to the permutation group G acting on the four spectral parameters β_ℓ, and using exactly the same arguments as we did from (78) through (81) we find :

$$\begin{array}{rcl} \int_0^\infty dw \int_0^{4\pi} dkwS_4^{+-}(w,k-\pi) = & & \int_0^{4\pi} dw \int_0^{4\pi} dkwS_4^{+-}(w,k-\pi) \\ & = & C_4 \int_{-\infty}^{+\infty} d\beta_1 ... \int_{-\infty}^{+\infty} d\beta_4 \\ & & \times\pi(\frac{1}{\cosh(\beta_1)} + \cdots + \frac{1}{\cosh(\beta_4)}) \\ & & \times F(\beta_1,\beta_2,\beta_3,\beta_4) \\ & & \times\sum_{\ell=1}^{2}\sum_{t\geq s\geq 0}^{\infty}[(3-2\delta_{1,\ell})(2-\delta_{s,t}) \\ & & \times Re\left(S_{1,\ell}^{s,t}(\beta_1,\ldots,\beta_4)\right)]. \end{array} \tag{84}$$

Again with the help of the Genz-Malik algorithm for the numeric integration of the latter integral we find :

$$\int_0^\infty dw \int_0^{4\pi} dkwS_4^{+-}(w,k-\pi) = 18.64 \pm 0.06, \tag{85}$$

which given the second sum rule (83) means that S_4^{+-} contributes 19.97% or almost 20% to the total S^{+-}. As a summary then the above two sum rules show that S_4^{+-} contributes between 18% and 20% to the total S^{+-}.

3.3 n-spinon

The general case of n-spinons parallels closely the case of 4-spinon. In particular the first sum rule (77) generalizes as :

$$\int_0^\infty dw \int_0^{n\pi} dkS^{i,+-}(w,k-\pi) = \frac{n}{2}\int_0^\infty dw \int_0^{2\pi} dkS^{i,+-}(w,k-\pi) = n\pi^2. \tag{86}$$

If we substitute S^{+-} by S_n^{+-} as given by (48) in the latter relation, and make a change of variables from (w,k) to $(\bar{\beta}_1,\bar{\beta}_2) \equiv (\beta_1,\beta_2)$ given by (43) as we did in the previous cases we find :

$$\begin{array}{rcl} \int_0^{n\pi} dw \int_0^{n\pi} dkS_n^{i,+-}(w,k-\pi) & = & C_{7,n}\int_{-\infty}^{+\infty} d\beta_1 \cdots \int_{-\infty}^{+\infty} d\beta_n F(\beta_1,\cdots,\beta_n) \\ & & \times\left(\sum_{\ell_{2N}\geq\ell_N,\ell_{2N-1},\ldots,\ell_1=1}^{n}\sum_{s_{2N},\ldots,s_1=0}^{\infty}(2-\delta_{\ell_{2N}\ell_N})\right. \\ & & \left.\times\ Re\left(S_{\ell_{2N},\ldots,\ell_1}^{s_{2N},\ldots,s_1}(\beta_1,\cdots,\beta_n)\right)\right), \end{array} \tag{87}$$

with N given by (19) and $C_{7,n}$ given by (49). With powerful enough computing resources one should be able to compute the latter integral numerically through the Genz-Malik algorithm at least for the cases $n = 6, 8, 10, 12$. Unfortunately we do not possess such computing resources and therefore we left this computation for the future when they become available to us. This would of course allow us to find the contribution of the n-spinon S_n^{+-} to the total S_n. The analogue of the second sum rule (83) in the case of n-spinon is :

$$\begin{array}{rcl} \int_0^\infty dw \int_0^{n\pi} dkwS^{i,+-}(w,k-\pi) & = & \frac{n}{2}\int_0^\infty dw \int_0^{2\pi} dkwS^{i,+-}(w,k-\pi) \\ & = & \frac{8ne_0\pi}{3}\int_0^{2\pi} dk(1-\cos(k)) \\ & = & \frac{16ne_0\pi^2}{3}. \end{array} \tag{88}$$

Similar derivation that led to (87) gives :

$$\begin{aligned}
\int_0^\infty dw \int_0^{n\pi} dkw S_n^{i,+-}(w,k-\pi) = & \int_0^{n\pi} dw \int_0^{n\pi} dkw S_n^{i,+-}(w,k-\pi) \\
= & \pi C_{7,n} \int_{-\infty}^{+\infty} d\beta_1 \cdots \int_{-\infty}^{+\infty} d\beta_n F(\beta_1,\cdots,\beta_n) \\
& \times(\cosh(\beta_1)^{-1} + \cdots + \cosh(\beta_n)^{-1}) \\
& \times \Big(\sum_{\ell_{2N}\geq\ell_N,\ell_{2N-1},\ldots,\ell_1=1}^{n} \sum_{s_{2N},\ldots,s_1=0}^{\infty} (2-\delta_{\ell_{2N}\ell_N}) \\
& \quad \times Re\left(S_{\ell_{2N},\ldots,\ell_1}^{s_{2N},\ldots,s_1}(\beta_1,\cdots,\beta_n)\right)\Big),
\end{aligned} \tag{89}$$

Again with powerful enough computing resources one should be able to evaluate the latter integrals a la Genz-Malik algorithm for at least $n = 6, 8, 10, 12$. Using the second sum rule (88) this would give us the contribution percentage of the n-spinon S_n^{+-} to the total S_n. This task is also left for the future computing resources permitting.

4 An approximation for the total DSF of the Heisenberg model

As mentionned in the introduction since in this paper we have shown that S_2 and S_4 saturate the total DSF only up to $54\% - 56\%$ we need therefore to study the higher sectors as well. From the shapes of S_2 in Figure 3 and S_4 in Figure 4 as functions of energy transfer for fixed momentum transfer one can notice that they are very similar in that S_4 almost looks like a scaled down version of S_2 in the common first Brouillin zone $[0, 2\pi]$. Beyond $[0, 2\pi]$ S_2 is null and S_4 is extremely small. One is tempted then to conclude that this pattern would still hold true for the general S_n. Since S_2 is the only one which is very simple and expressed as a single term and captures the general shape of the general S_n up to a scale factor we propose then an approximation to the total DSF as scaled up version of S_2 such that it saturates the sum rules. This approximation is somewhere in the middle between the Muller ansatz and the exact one. It's better than the Muller anstaz because it has a much better shape that closely fits the experimental data and it is almost as simple as the Muller anstaz, and also it is much simpler that the exact total DSF which is very complex. The only drawback is that it misses all the spectral weight beyond the first Brouillin zone of $[0, 2\pi]$ although the latter is negligeable for general n. To recap if we rescale the overall factor to saturate the sum rules we find then the approxiamte total DSF of the Heisenberg model to be

$$S_{Approx}^{xx}(w,k-\pi) = S_{Approx}^{yy}(w,k-\pi) = S_{Approx}^{zz}(w,k-\pi) = \frac{25}{18} S_2^{+-}(w,k-\pi). \tag{90}$$

S_{Approx}^{zz} is plotted in Figure 6 as a function of w for fixed $k = \pi$.

5 Conclusion

In this paper we have derived the n-spinon DSF S_n and we have proved why any sector among the two possible sectors of the eisengspace should be considered but not both at the same time. This allowed us to correct the overall factors in the existing formulas in the litterature. In particular we have shown that the overall factor of the n-spinon DSF can be expressed in terms of the Glaisher-Kinkelin constant. We have extensively studied the 2-spinon and 4-spinon cases and in particular we have shown that the 2-spinon DSF accounts for 36% of the total DSF and that the 4-spinon DSF account for between 18% and 20% for the total DSF depending on the sum rule. In the case of 4-spinon we have derived a set of highly nontrivial symmetry relations

involving permutations of the spectral parameters and indices of the DSF terms. It begs the question whether the latter symmetry relations can be generalized to the n-spinon case. We have derived analytically the integrals corresponding to the sum rules for the general case of n-spinon and all it remains is to evaluate them numerically at least for the cases $n = 6, 8, 10, 12$ using the Genz-Malik algorithm or any other one. We have proposed an approximation to the total DSF based on rescaling the overall factor of the 2-spinon DSF such that it saturates the sum rules. Finally we propose as an experiment to detect any non vanishing S for fixed k and w greater than $W_u = 2\pi \sin(k/2)$ of the 2-spinon case which would signal the presence of 4 spinons and higher in the spectrum.

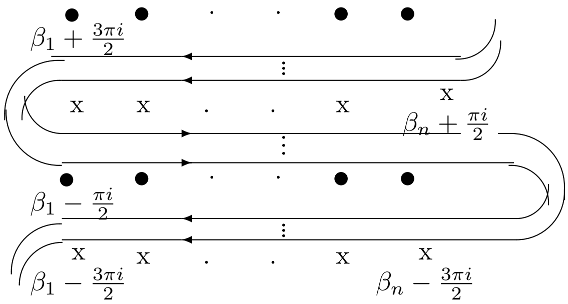

Figure 1. : The $\frac{n-2}{2}$ contours $\bar{C}_n$ used in the n-spinon case

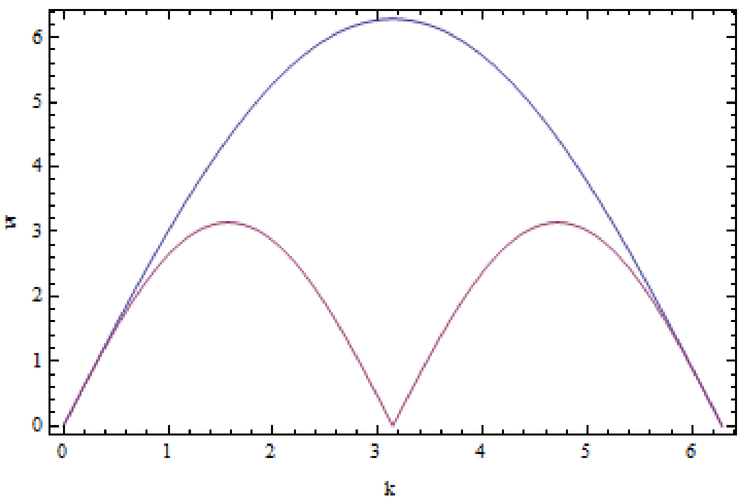

Figure 2. : Dispersion relation in the 2-spinon case

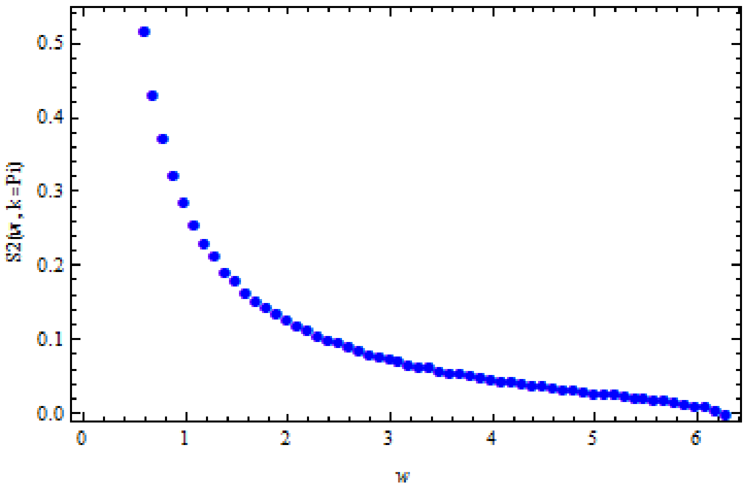

Figure 3. : S_2 as a function of w for fixed $k = \pi$

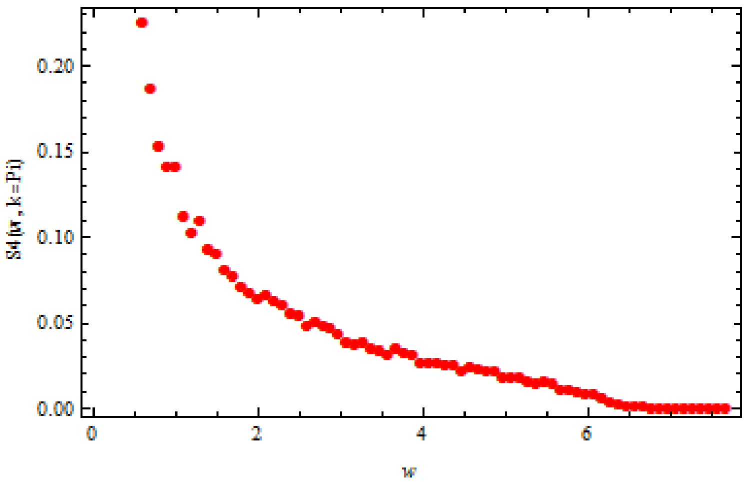

Figure 4. : S_4 as a function of w for fixed $k = \pi$

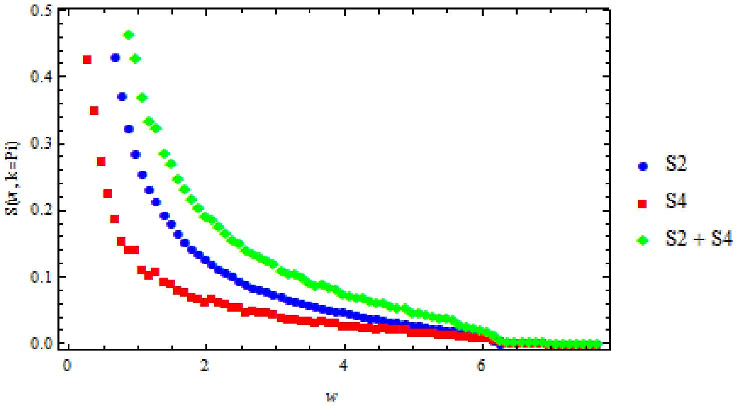

Figure 5. : $S_2 + S_4$ as a function of w for fixed $k = \pi$

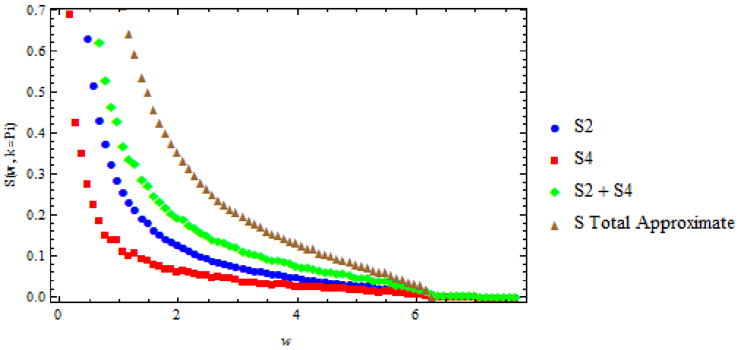

Figure 6. : S Total Approximate as a function of w for fixed $k = \pi$

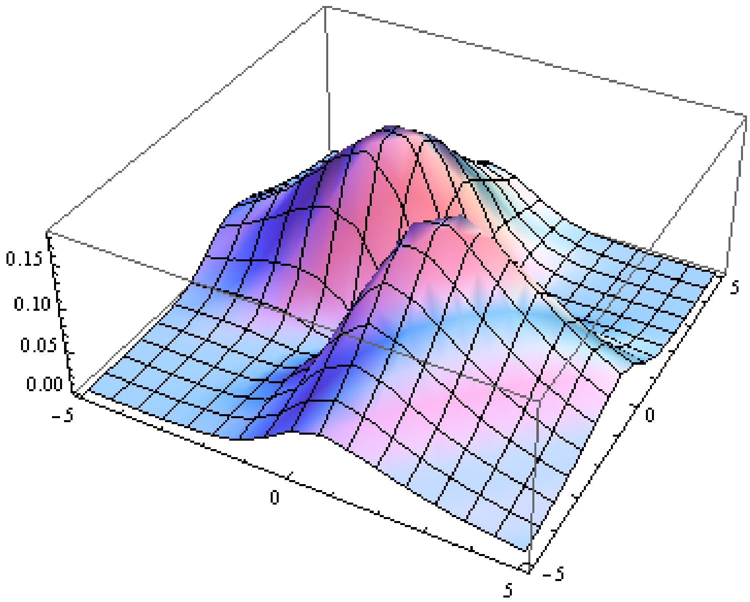

Figure 7. : Plot of the 2-spinon integrand of the total integrated intensity sum rule as a function of β_1 and β_2

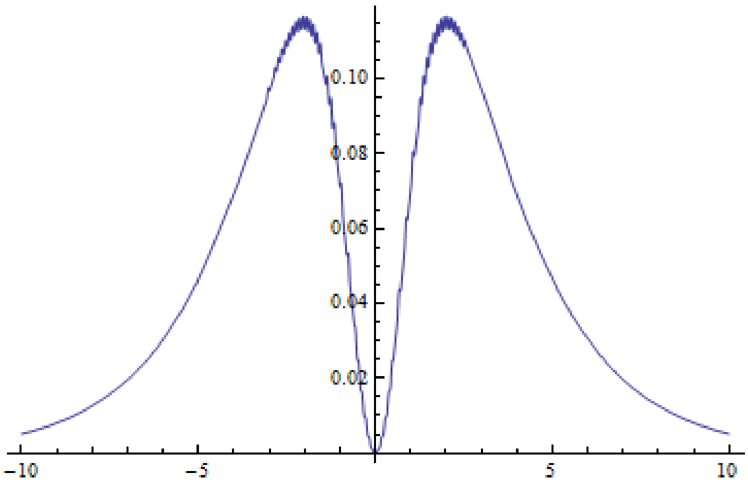

Figure 8. : Plot of the 2-spinon integrand of the total integrated intensity sum rule as a function of β_1 for fixed $\beta_2 = 0$

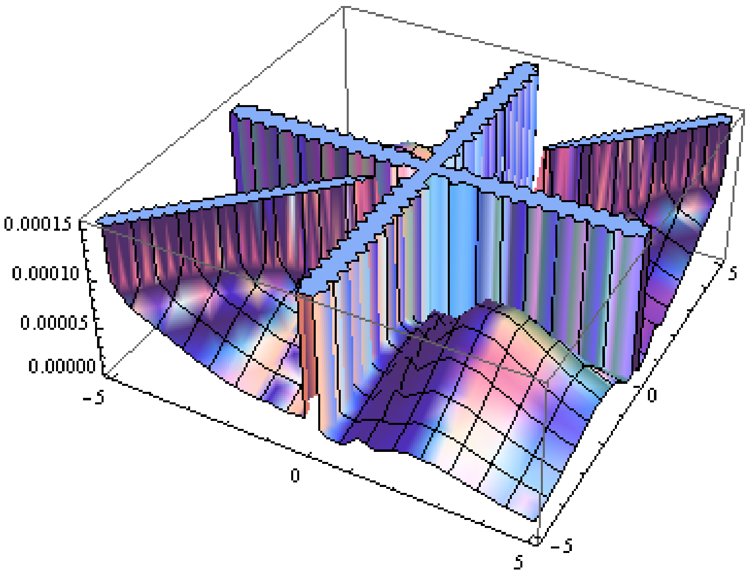

Figure 9. : Plot of the 4-spinon integrand of the total integrated intensity sum rule as a function of β_1 and β_2 for fixed $\beta_3 = 0$ and $\beta_4 = 1$

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